



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 PM UTC

PDB ID : 5BKL / pdb_00005bkl
Title : Crystallographic structure of the cubic crystal form of STMV (77.9 degree rotation) grown from NaCl
Authors : McPherson, A.
Deposited on : 2021-03-20
Resolution : 2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

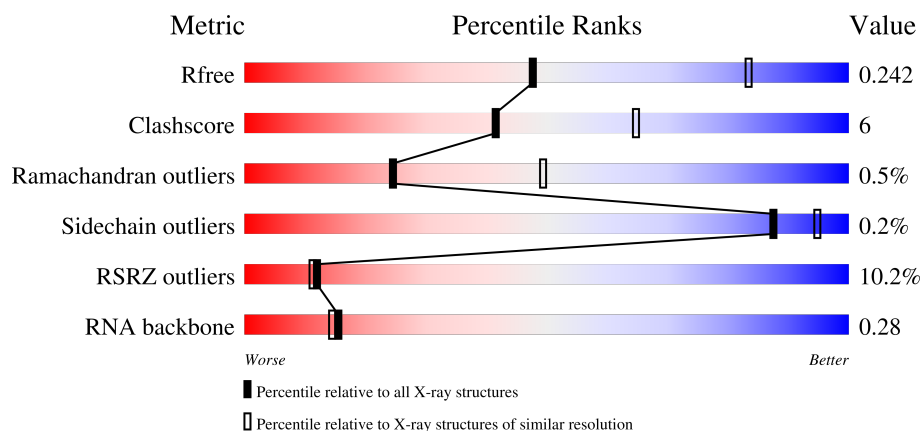
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)
RNA backbone	3983	1018 (3.14-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	5% 81% 9% • 9%
1	B	159	4% 78% 11% • 10%
1	C	159	3% 82% 6% • 11%
1	D	159	3% 82% 8% • 9%

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Mol	Chain	Length	Quality of chain
1	E	159	
1	F	159	
1	G	159	
1	GG	159	
1	H	159	
1	HH	159	
1	I	159	
1	II	159	
1	J	159	
1	JJ	159	
1	K	159	
1	KK	159	
1	L	159	
1	M	159	
1	N	159	
1	O	159	
2	P	12	
2	S	12	
2	T	12	
2	UU	12	
2	V	12	
2	X	12	
2	bb	12	
3	TT	11	
3	Y	11	

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Mol	Chain	Length	Quality of chain
3	a	11	
4	WW	13	
4	e	13	
4	h	13	
4	i	13	
4	kk	13	
4	ll	13	
4	n	13	
4	qq	13	
5	m	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	B	303	-	-	X	-
6	CL	B	304	-	-	X	-
6	CL	C	206	-	-	X	-
6	CL	F	201	-	-	X	-
6	CL	G	301	-	-	X	-
6	CL	H	201	-	-	X	-
6	CL	H	202	-	-	X	-
6	CL	II	202	-	-	X	-
6	CL	JJ	302	-	-	X	-
6	CL	KK	201	-	-	X	-
7	MG	K	303	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50583 atoms, of which 23747 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	S	2	13	0
			2292	721	1147	204	213	7			
1	B	143	Total	C	H	N	O	S	0	12	0
			2212	703	1097	197	208	7			
1	C	142	Total	C	H	N	O	S	2	21	0
			2223	701	1110	198	208	6			
1	D	144	Total	C	H	N	O	S	1	21	0
			2259	711	1132	199	210	7			
1	E	144	Total	C	H	N	O	S	0	19	0
			2241	712	1109	200	213	7			
1	F	144	Total	C	H	N	O	S	0	17	0
			2298	723	1152	202	214	7			
1	G	146	Total	C	H	N	O	S	2	15	0
			2268	720	1124	202	215	7			
1	H	145	Total	C	H	N	O	S	1	14	0
			2248	711	1117	200	213	7			
1	I	144	Total	C	H	N	O	S	0	13	0
			2259	711	1130	200	211	7			
1	J	147	Total	C	H	N	O	S	0	15	0
			2302	732	1138	205	220	7			
1	K	145	Total	C	H	N	O	S	1	16	0
			2356	739	1181	211	219	6			
1	L	157	Total	C	H	N	O	S	14	15	0
			2465	800	1194	227	236	8			
1	M	144	Total	C	H	N	O	S	0	13	0
			2366	740	1194	207	218	7			
1	N	144	Total	C	H	N	O	S	1	13	0
			2329	730	1172	201	217	9			
1	O	150	Total	C	H	N	O	S	0	23	0
			2296	735	1123	209	222	7			
1	GG	145	Total	C	H	N	O	S	1	19	0
			2254	711	1123	200	213	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HH	145	Total	C	H	N	O	S	0	15	0
			2295	724	1145	204	215	7			
1	II	143	Total	C	H	N	O	S	0	16	0
			2238	710	1112	198	210	8			
1	JJ	144	Total	C	H	N	O	S	0	16	0
			2230	703	1112	199	210	6			
1	KK	144	Total	C	H	N	O	S	0	10	0
			2210	707	1087	199	210	7			

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	7	Total 220	C 70	H 66	N 35	O 42	P 7	0	7	0
2	S	7	Total 209	C 70	H 55	N 35	O 42	P 7	0	6	0
2	T	5	Total 156	C 50	H 46	N 25	O 30	P 5	0	5	0
2	V	8	Total 233	C 80	H 57	N 40	O 48	P 8	0	6	0
2	X	8	Total 264	C 80	H 88	N 40	O 48	P 8	0	8	0
2	UU	7	Total 215	C 70	H 61	N 35	O 42	P 7	0	7	0
2	bb	11	Total 314	C 110	H 72	N 55	O 66	P 11	0	8	0

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Y	9	Total	C	H	N	O	P	0	6	0
			258	90	60	45	54	9			
3	a	5	Total	C	H	N	O	P	0	5	0
			165	50	55	25	30	5			
3	TT	6	Total	C	H	N	O	P	0	4	0
			171	60	39	30	36	6			

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	e	11	Total 300	C 99	H 80	N 22	O 88	P 11	0	10	0
4	h	7	Total 198	C 63	H 58	N 14	O 56	P 7	0	7	0
4	i	5	Total 140	C 45	H 40	N 10	O 40	P 5	0	5	0
4	n	7	Total 198	C 63	H 58	N 14	O 56	P 7	0	7	0
4	WW	10	Total 211	C 90	H 11	N 20	O 80	P 10	0	2	0
4	kk	6	Total 160	C 54	H 40	N 12	O 48	P 6	0	5	0
4	ll	5	Total 140	C 45	H 40	N 10	O 40	P 5	0	5	0
4	qq	6	Total 152	C 54	H 32	N 12	O 48	P 6	0	4	0

- Molecule 5 is a RNA chain called RNA (5'-R(UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	m	9	Total	C	H	N	O	P	0	9	0
			270	81	90	18	72	9			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cl	0	0
			4	4		
6	C	6	Total	Cl	0	0
			6	6		
6	D	2	Total	Cl	0	0
			2	2		
6	F	2	Total	Cl	0	0
			2	2		
6	G	2	Total	Cl	0	0
			2	2		
6	H	2	Total	Cl	0	0
			2	2		
6	K	2	Total	Cl	0	0
			2	2		
6	L	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	1	Total 1	Cl 1	0	0
6	GG	1	Total 1	Cl 1	0	0
6	HH	2	Total 2	Cl 2	0	0
6	II	3	Total 3	Cl 3	0	0
6	JJ	5	Total 5	Cl 5	0	0
6	KK	5	Total 5	Cl 5	0	0
6	TT	1	Total 1	Cl 1	0	0
6	ll	1	Total 1	Cl 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	2	Total 2	Mg 2	0	0
7	F	2	Total 2	Mg 2	0	0
7	G	1	Total 1	Mg 1	0	0
7	I	1	Total 1	Mg 1	0	0
7	K	1	Total 1	Mg 1	0	0
7	GG	1	Total 1	Mg 1	0	0
7	HH	2	Total 2	Mg 2	0	0
7	JJ	2	Total 2	Mg 2	0	0
7	KK	1	Total 1	Mg 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	25	Total O 25 25	0	0
8	B	32	Total O 32 32	0	0
8	C	41	Total O 41 41	0	0
8	D	53	Total O 53 53	0	0
8	E	19	Total O 19 19	0	0
8	F	24	Total O 24 24	0	0
8	G	37	Total O 37 37	0	0
8	H	23	Total O 23 23	0	0
8	I	24	Total O 24 24	0	0
8	J	21	Total O 21 21	0	0
8	K	24	Total O 24 24	0	0
8	L	16	Total O 16 16	0	0
8	M	16	Total O 16 16	0	0
8	N	14	Total O 14 14	0	0
8	O	49	Total O 49 49	0	0
8	P	4	Total O 4 4	0	0
8	S	14	Total O 14 14	0	0
8	T	4	Total O 4 4	0	0
8	V	19	Total O 19 19	0	0
8	X	3	Total O 3 3	0	0
8	Y	10	Total O 10 10	0	0
8	a	8	Total O 8 8	0	0

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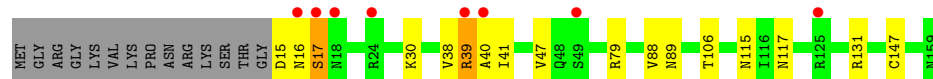
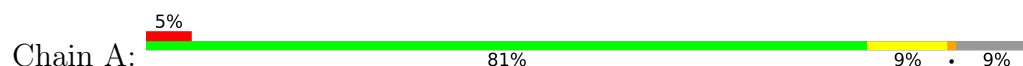
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	e	40	Total O 40 40	0	0
8	h	9	Total O 9 9	0	0
8	i	5	Total O 5 5	0	0
8	m	7	Total O 7 7	0	0
8	n	8	Total O 8 8	0	0
8	GG	38	Total O 38 38	0	0
8	HH	60	Total O 60 60	0	0
8	II	60	Total O 60 60	0	0
8	JJ	54	Total O 54 54	0	0
8	KK	54	Total O 54 54	0	0
8	TT	9	Total O 9 9	0	0
8	UU	14	Total O 14 14	0	0
8	WW	10	Total O 10 10	0	0
8	bb	42	Total O 42 42	0	0
8	kk	7	Total O 7 7	0	0
8	ll	9	Total O 9 9	0	0
8	qq	9	Total O 9 9	0	0

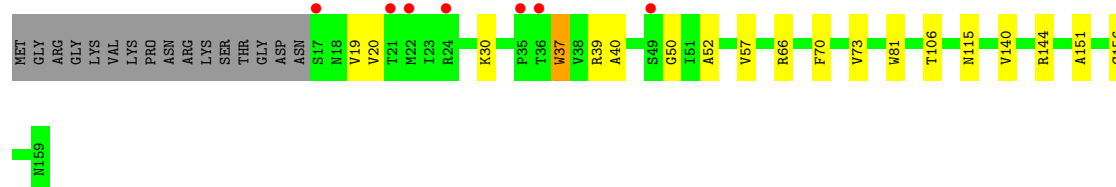
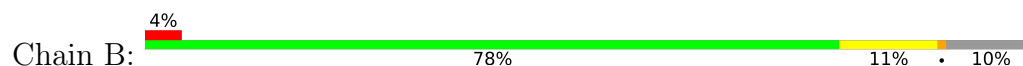
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

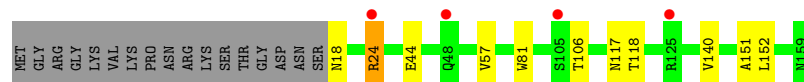
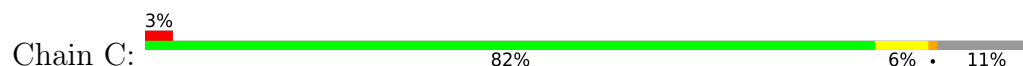
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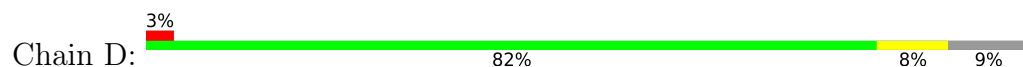
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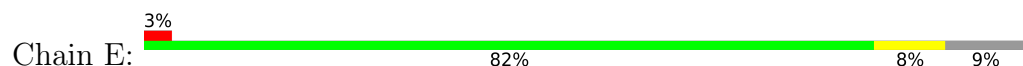
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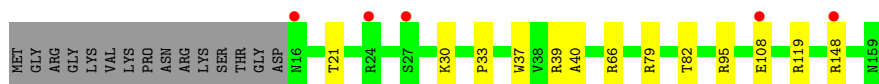


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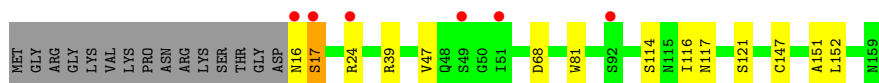
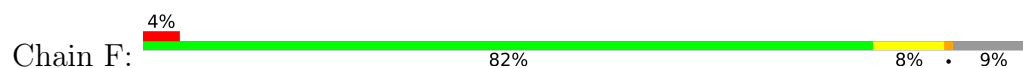


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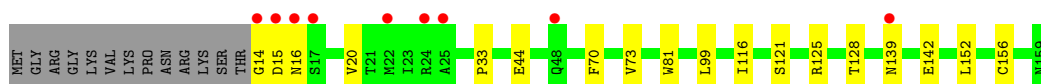
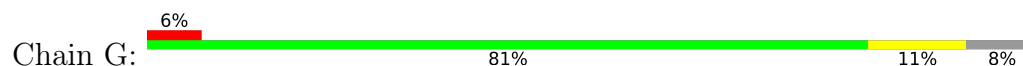




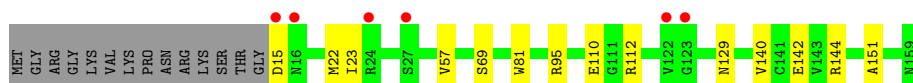
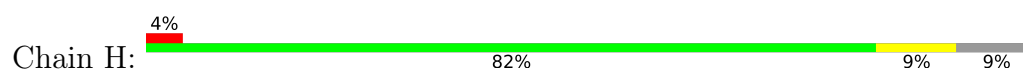
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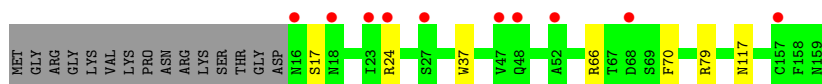
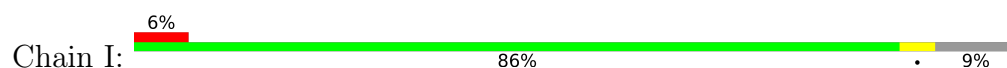
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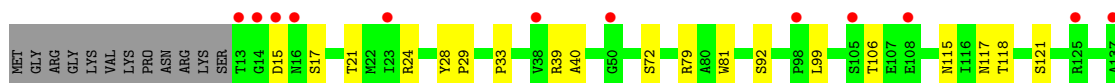
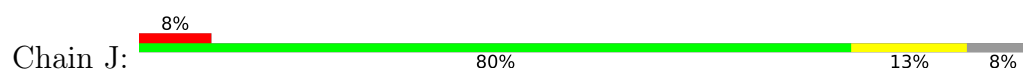
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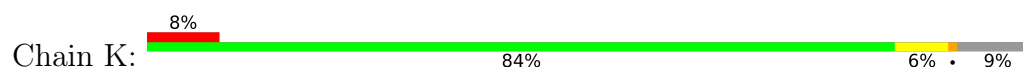
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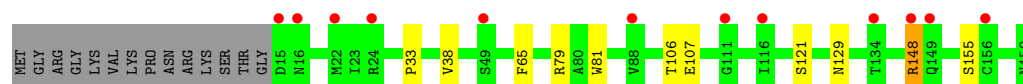


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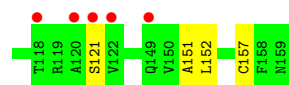
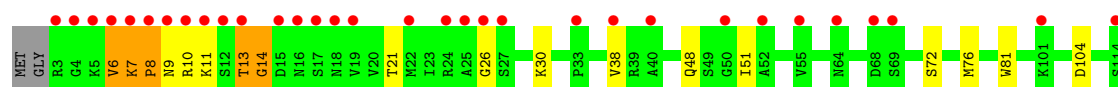
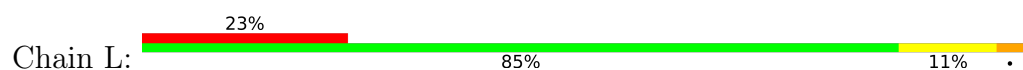


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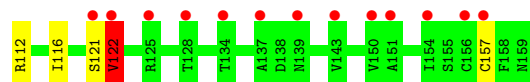
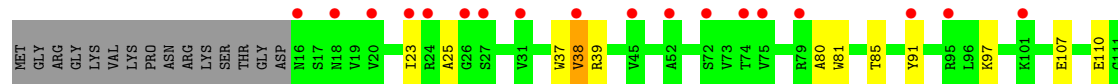
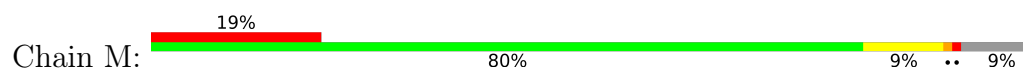




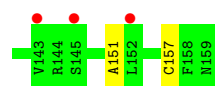
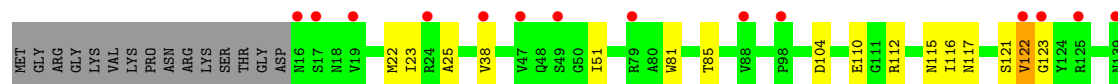
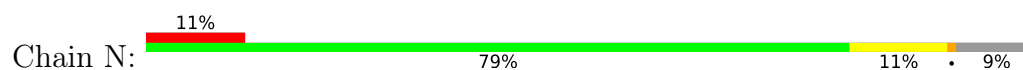
• Molecule 1: Coat protein



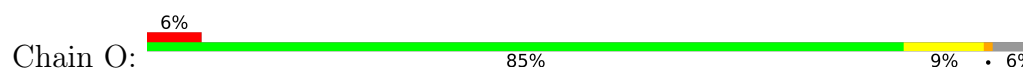
• Molecule 1: Coat protein



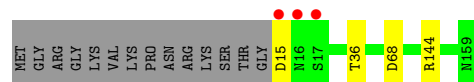
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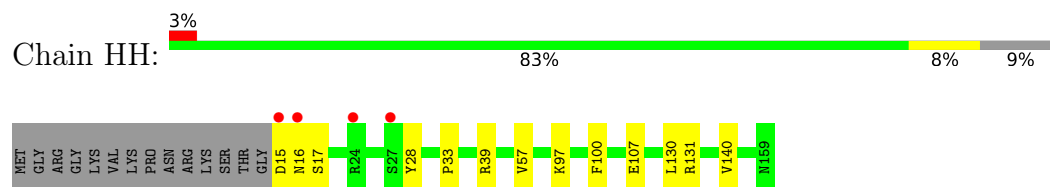
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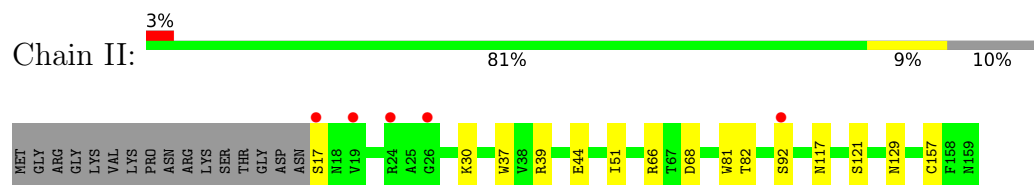
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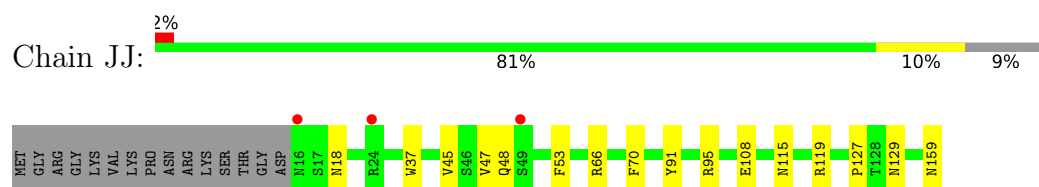
- Molecule 1: Coat protein



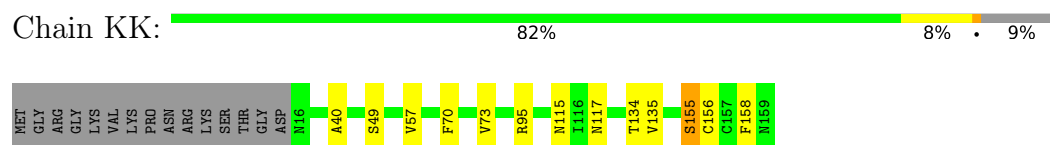
- Molecule 1: Coat protein



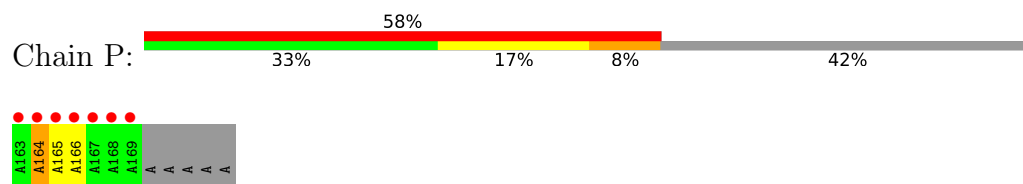
- Molecule 1: Coat protein



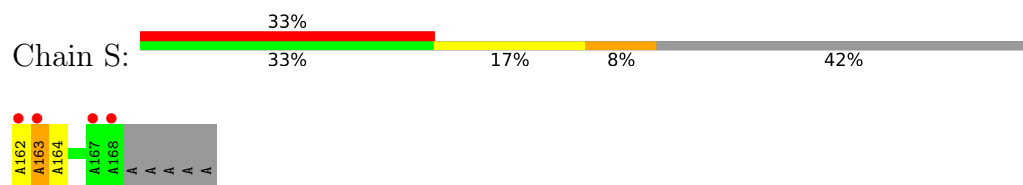
- Molecule 1: Coat protein



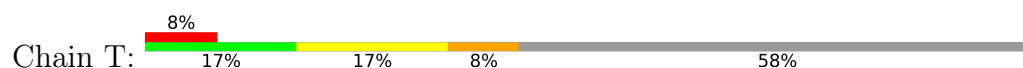
- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

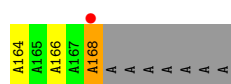


- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

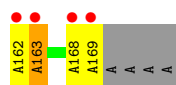
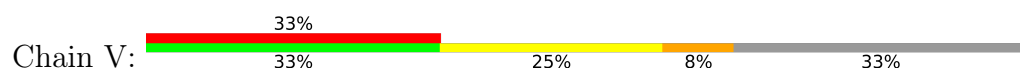


- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

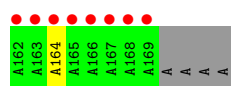




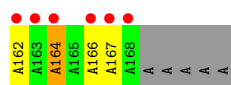
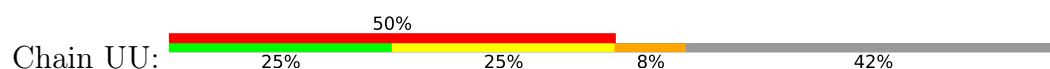
- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



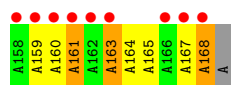
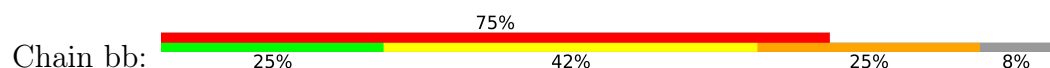
- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



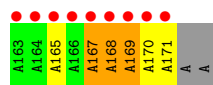
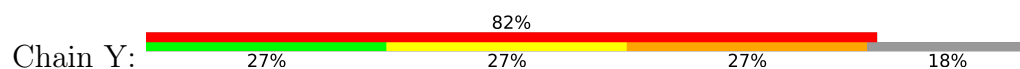
- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



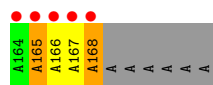
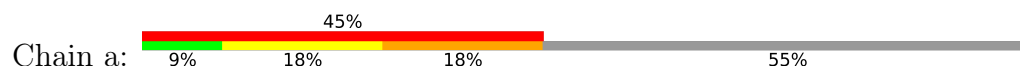
- Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



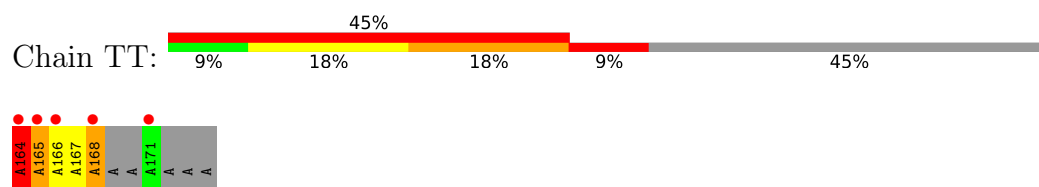
- Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



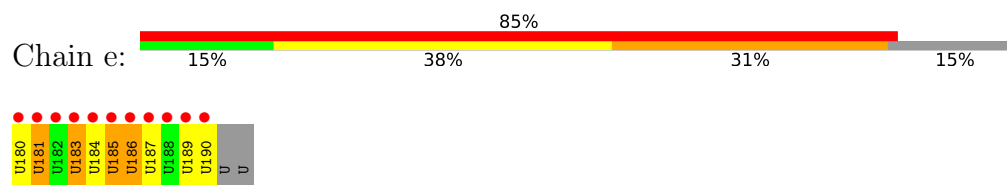
- Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



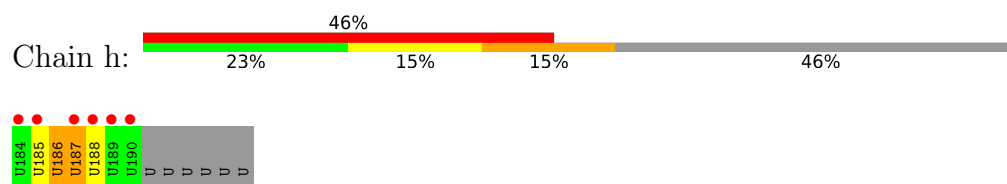
- Molecule 3: RNA (5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



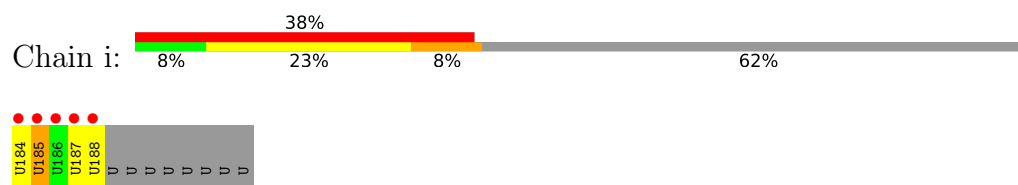
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



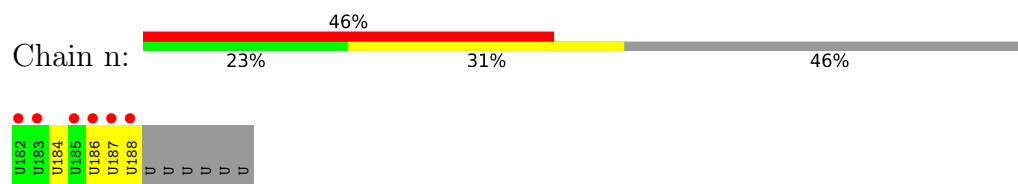
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



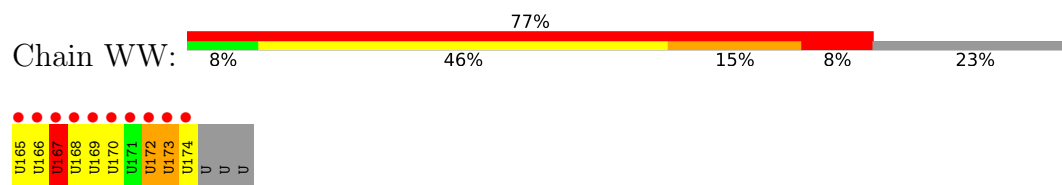
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



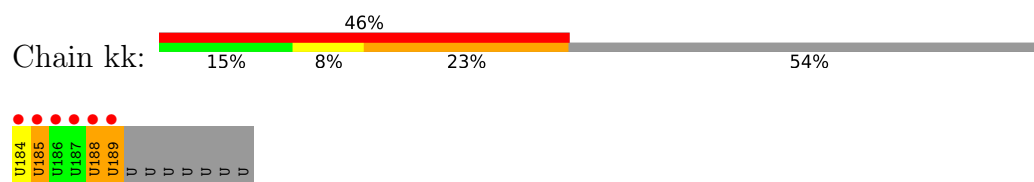
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



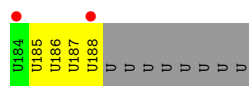
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



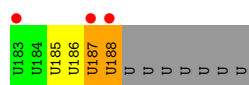
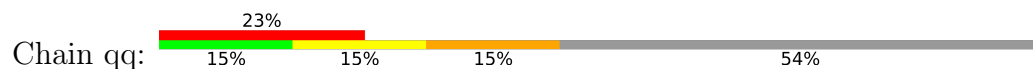
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



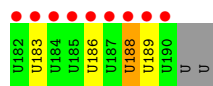
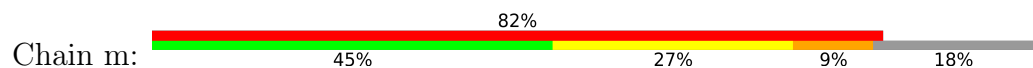
- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 4: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 5: RNA (5'-R(UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	234.65Å 234.65Å 234.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.22 – 2.94 78.22 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.4 (78.22-2.94) 80.9 (78.22-2.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.217 , 0.256 0.207 , 0.242	Depositor DCC
R_{free} test set	4399 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	50583	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/1193	0.30	0/1623
1	B	0.15	0/1154	0.31	0/1571
1	C	0.16	0/1153	0.32	0/1571
1	D	0.16	0/1192	0.31	0/1624
1	E	0.17	0/1186	0.33	0/1614
1	F	0.13	0/1222	0.29	0/1665
1	G	0.15	0/1205	0.29	0/1641
1	GG	0.17	0/1174	0.33	0/1599
1	H	0.15	0/1179	0.31	0/1606
1	HH	0.15	0/1205	0.31	0/1641
1	I	0.14	0/1167	0.29	0/1589
1	II	0.17	0/1198	0.33	0/1630
1	J	0.14	0/1223	0.30	0/1664
1	JJ	0.16	0/1142	0.32	0/1556
1	K	0.15	0/1263	0.31	0/1720
1	KK	0.17	0/1150	0.32	0/1566
1	L	0.20	0/1358	0.41	0/1844
1	M	0.13	0/1248	0.31	0/1697
1	N	0.12	0/1241	0.30	0/1689
1	O	0.15	0/1203	0.31	0/1636
2	P	0.23	0/174	0.49	0/269
2	S	0.10	0/174	0.19	0/269
2	T	0.13	0/124	0.27	0/191
2	UU	0.14	0/174	0.36	0/269
2	V	0.11	0/199	0.27	0/308
2	X	0.11	0/199	0.30	0/308
2	bb	0.16	0/274	0.32	0/425
3	TT	0.92	1/148 (0.7%)	1.15	1/226 (0.4%)
3	Y	0.21	0/224	0.96	2/347 (0.6%)
3	a	0.39	0/124	0.93	0/191
4	WW	0.39	0/219	1.25	6/336 (1.8%)
4	e	0.23	0/241	0.66	0/370

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	h	0.13	0/153	0.41	0/234
4	i	0.16	0/109	0.43	0/166
4	kk	0.26	0/131	0.69	0/200
4	ll	0.16	0/109	0.34	0/166
4	n	0.12	0/153	0.31	0/234
4	qq	0.24	0/131	0.66	0/200
5	m	0.12	0/197	0.29	0/302
All	All	0.18	1/27313 (0.0%)	0.37	9/37757 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	1
1	GG	0	1
1	K	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	TT	164[A]	A	C4'-C3'	5.17	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	WW	166[A]	U	OP1-P-O3'	-9.62	79.15	108.00
3	Y	167[A]	A	OP1-P-O3'	-9.28	80.15	108.00
4	WW	167[A]	U	O5'-C5'-C4'	8.81	124.72	111.50
3	Y	167[A]	A	OP2-P-O3'	-8.08	83.77	108.00
4	WW	166[A]	U	OP2-P-O3'	-7.60	85.19	108.00
4	WW	167[A]	U	P-O5'-C5'	7.02	131.43	120.90
4	WW	166[A]	U	O3'-P-O5'	-6.10	94.85	104.00
4	WW	167[A]	U	C5'-C4'-C3'	5.19	123.79	116.00
3	TT	164[A]	A	C3'-C2'-O2'	5.15	118.42	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39[A]	ARG	Sidechain
1	A	39[B]	ARG	Sidechain
1	C	24	ARG	Sidechain
1	E	148	ARG	Sidechain
1	GG	144	ARG	Sidechain
1	K	148[A]	ARG	Sidechain
1	K	148[B]	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1145	1147	1113	16	1
1	B	1115	1097	1093	14	0
1	C	1113	1110	1048	10	0
1	D	1127	1132	1066	15	0
1	E	1132	1109	1071	11	0
1	F	1146	1152	1085	11	0
1	G	1144	1124	1095	19	0
1	GG	1131	1123	1057	4	0
1	H	1131	1117	1078	12	1
1	HH	1150	1145	1113	13	0
1	I	1129	1130	1096	7	0
1	II	1126	1112	1085	14	0
1	J	1164	1138	1130	18	0
1	JJ	1118	1112	1078	13	0
1	K	1175	1181	1125	14	0
1	KK	1123	1087	1105	14	0
1	L	1271	1194	1264	20	2
1	M	1172	1194	1177	9	1
1	N	1157	1172	1135	11	1
1	O	1173	1123	1118	20	0
2	P	154	66	78	5	0
2	S	154	55	78	3	1
2	T	110	46	56	6	0
2	UU	154	61	78	6	0
2	V	176	57	89	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	176	88	89	0	1
2	bb	242	72	122	11	1
3	TT	132	39	68	5	0
3	Y	198	60	100	7	0
3	a	110	55	56	6	0
4	WW	200	11	95	7	0
4	e	220	80	111	12	1
4	h	140	58	71	9	0
4	i	100	40	51	11	0
4	kk	120	40	61	6	0
4	ll	100	40	51	5	1
4	n	140	58	71	6	0
4	qq	120	32	61	14	0
5	m	180	90	91	3	0
6	B	4	0	0	4	0
6	C	6	0	0	3	0
6	D	2	0	0	2	0
6	F	2	0	0	3	0
6	G	2	0	0	2	0
6	GG	1	0	0	0	0
6	H	2	0	0	8	0
6	HH	2	0	0	1	0
6	II	3	0	0	4	0
6	JJ	5	0	0	4	0
6	K	2	0	0	1	0
6	KK	5	0	0	5	0
6	L	1	0	0	1	0
6	T	1	0	0	0	0
6	TT	1	0	0	0	1
6	ll	1	0	0	0	0
7	E	2	0	0	0	0
7	F	2	0	0	0	0
7	G	1	0	0	0	0
7	GG	1	0	0	0	0
7	HH	2	0	0	0	0
7	I	1	0	0	0	0
7	JJ	2	0	0	0	0
7	K	1	0	0	0	0
7	KK	1	0	0	0	0
8	A	25	0	0	0	0
8	B	32	0	0	1	1
8	C	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	53	0	0	1	0
8	E	19	0	0	1	0
8	F	24	0	0	1	0
8	G	37	0	0	1	0
8	GG	38	0	0	1	0
8	H	23	0	0	1	0
8	HH	60	0	0	0	0
8	I	24	0	0	0	1
8	II	60	0	0	4	1
8	J	21	0	0	1	0
8	JJ	54	0	0	3	1
8	K	24	0	0	0	0
8	KK	54	0	0	0	1
8	L	16	0	0	1	0
8	M	16	0	0	0	0
8	N	14	0	0	0	1
8	O	49	0	0	1	0
8	P	4	0	0	0	0
8	S	14	0	0	1	0
8	T	4	0	0	0	0
8	TT	9	0	0	1	0
8	UU	14	0	0	0	0
8	V	19	0	0	1	0
8	WW	10	0	0	0	0
8	X	3	0	0	0	0
8	Y	10	0	0	0	0
8	a	8	0	0	1	0
8	bb	42	0	0	3	0
8	e	40	0	0	0	0
8	h	9	0	0	2	0
8	i	5	0	0	0	0
8	kk	7	0	0	0	0
8	ll	9	0	0	0	0
8	m	7	0	0	1	0
8	n	8	0	0	1	0
8	qq	9	0	0	2	0
All	All	26836	23747	23609	309	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:GG:306:HOH:O	6:KK:201:CL:CL	2.01	1.14
8:II:309:HOH:O	6:KK:201:CL:CL	2.02	1.11
6:F:202:CL:CL	8:F:308:HOH:O	2.04	1.09
1:K:79[B]:ARG:NH2	3:Y:169:A:OP1	1.86	1.09
1:KK:155[A]:SER:OG	4:qq:188:U:OP1	1.71	1.08
6:B:304:CL:CL	8:E:306:HOH:O	2.09	1.05
1:GG:15:ASP:N	4:kk:184[A]:U:HO2'	1.57	1.03
1:B:39:ARG:NH2	6:B:303:CL:CL	2.33	0.98
6:B:304:CL:CL	8:C:323:HOH:O	2.19	0.97
1:L:6:VAL:HG13	1:L:7:LYS:H	1.27	0.96
2:UU:164[A]:A:N6	4:ll:185[A]:U:O4	2.00	0.94
2:UU:162[A]:A:H61	4:ll:187[A]:U:H3	1.11	0.93
1:C:18:ASN:N	6:C:203:CL:CL	2.41	0.90
1:A:39[B]:ARG:NH2	1:O:32:ASN:O	2.06	0.88
1:A:79:ARG:NH2	4:e:187[A]:U:OP1	2.07	0.87
3:a:167[A]:A:O4'	8:a:201:HOH:O	1.93	0.86
1:G:14:GLY:N	2:UU:162[A]:A:HO2'	1.72	0.86
1:L:6:VAL:O	1:L:7:LYS:HG2	1.78	0.83
4:qq:188:U:O2	4:qq:188:U:H2'	1.79	0.83
4:qq:188:U:O2'	8:qq:201:HOH:O	1.95	0.83
4:e:185[A]:U:O2'	4:e:186[A]:U:O4'	1.98	0.82
1:L:6:VAL:HG13	1:L:7:LYS:N	1.94	0.81
1:A:16:ASN:OD1	1:A:17:SER:N	2.14	0.81
4:WW:167[A]:U:H2'	4:WW:168:U:O5'	1.81	0.81
1:O:14:GLY:HA3	4:i:184[A]:U:P	2.21	0.80
8:II:319:HOH:O	6:KK:201:CL:CL	2.37	0.79
2:S:163[A]:A:O2'	8:S:201:HOH:O	1.94	0.79
1:I:79:ARG:NH2	5:m:188[A]:U:OP1	2.17	0.78
1:GG:15:ASP:N	4:kk:184[A]:U:O2'	2.17	0.77
1:G:20:VAL:O	8:G:401:HOH:O	2.02	0.76
1:JJ:119:ARG:O	8:JJ:401:HOH:O	2.04	0.76
1:O:108:GLU:O	8:O:201:HOH:O	2.03	0.75
6:G:301:CL:CL	1:HH:28:TYR:OH	2.41	0.74
1:L:152:LEU:O	8:L:601:HOH:O	2.05	0.74
4:h:187[A]:U:OP1	8:h:201:HOH:O	2.05	0.73
1:K:148[B]:ARG:HG2	1:K:148[B]:ARG:HH11	1.53	0.73
1:G:14:GLY:N	2:UU:162[A]:A:O2'	2.22	0.72
2:bb:163[A]:A:H2	4:qq:187[A]:U:H3	1.35	0.72
1:G:16:ASN:ND2	6:HH:402:CL:CL	2.59	0.72
1:E:79:ARG:NH2	4:i:188[A]:U:OP1	2.22	0.72
1:L:11:LYS:HB2	1:L:21:THR:HG21	1.73	0.71
4:WW:167[A]:U:C2'	4:WW:168:U:O5'	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:SER:OG	8:H:301:HOH:O	2.09	0.70
2:UU:162[A]:A:N6	4:ll:187[A]:U:H3	1.88	0.69
1:J:21:THR:HG22	2:P:165[A]:A:H5''	1.74	0.69
5:m:186[A]:U:O4'	8:m:201:HOH:O	2.11	0.69
1:J:17:SER:HA	2:P:164[A]:A:H4'	1.76	0.68
1:KK:40:ALA:HB2	4:qq:187[A]:U:H4'	1.73	0.68
1:II:39:ARG:NH2	6:II:201:CL:CL	2.64	0.67
4:e:180:U:H1'	4:e:181[A]:U:OP1	1.94	0.67
1:GG:36:THR:OG1	4:ll:185[A]:U:O2'	2.11	0.66
1:N:38:VAL:HG22	1:N:157[B]:CYS:SG	2.36	0.66
4:WW:172:U:OP2	4:WW:172:U:H2'	1.96	0.65
4:n:188[A]:U:O5'	8:n:201:HOH:O	2.15	0.65
2:bb:161[A]:A:N6	8:bb:201:HOH:O	2.28	0.65
2:UU:166[A]:A:H2'	2:UU:167[A]:A:O4'	1.96	0.65
1:L:6:VAL:O	1:L:7:LYS:CG	2.45	0.64
1:II:82:THR:HG21	1:II:92[B]:SER:OG	1.97	0.64
1:H:129:ASN:ND2	1:HH:131:ARG:O	2.26	0.64
1:M:121:SER:O	1:M:122:VAL:HG12	1.97	0.64
1:JJ:159:ASN:OXT	8:JJ:402:HOH:O	2.15	0.63
4:e:185[A]:U:O2'	4:e:186[A]:U:H5''	1.98	0.63
1:J:28:TYR:OH	6:K:302:CL:CL	2.48	0.62
2:V:168[A]:A:N3	8:V:201:HOH:O	2.31	0.62
1:A:39[B]:ARG:HG2	1:A:41:ILE:HD11	1.82	0.61
1:B:40:ALA:O	6:B:303:CL:CL	2.56	0.61
4:qq:187[A]:U:O2'	4:qq:188:U:H5'	2.01	0.61
1:J:92:SER:OG	8:J:201:HOH:O	2.16	0.60
1:N:121:SER:O	1:N:122:VAL:HG12	2.02	0.60
1:O:11:LYS:HE3	2:T:168[A]:A:N1	2.16	0.60
1:H:95:ARG:HD3	6:H:202:CL:CL	2.38	0.60
1:O:14:GLY:HA2	4:i:184[A]:U:H4'	1.82	0.60
1:A:40:ALA:HB2	4:e:186[A]:U:H4'	1.84	0.59
2:P:165[A]:A:C2	4:e:185[A]:U:O4	2.55	0.59
1:L:6:VAL:CG1	1:L:7:LYS:N	2.66	0.58
4:kk:188[A]:U:H2'	4:kk:189:U:H5'	1.86	0.57
1:E:40:ALA:HB2	4:i:187[A]:U:H4'	1.84	0.57
1:KK:95:ARG:HD3	6:KK:203:CL:CL	2.41	0.57
1:A:39[B]:ARG:NH2	1:A:40:ALA:O	2.38	0.57
2:T:164[A]:A:H5'	1:HH:16:ASN:HB3	1.86	0.57
4:i:184[A]:U:O2'	4:i:185[A]:U:OP1	2.21	0.57
4:h:187[A]:U:O2'	8:h:202:HOH:O	2.17	0.57
1:D:79:ARG:NE	6:D:202:CL:CL	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:202:CL:CL	1:HH:33:PRO:CD	2.90	0.56
1:D:127:PRO:HB3	1:II:17:SER:O	2.06	0.56
2:bb:163[A]:A:N1	4:qq:187[A]:U:O4	2.39	0.56
1:D:110:GLU:OE1	8:D:301:HOH:O	2.17	0.56
4:h:187[A]:U:H5'	6:II:202:CL:CL	2.43	0.56
1:H:144:ARG:NE	6:H:201:CL:CL	2.74	0.56
1:J:99:LEU:HG	1:J:141:CYS:HA	1.88	0.56
2:S:162:A:H1'	2:S:163[A]:A:C8	2.41	0.55
1:D:18:ASN:HA	1:II:129:ASN:HD21	1.73	0.54
3:a:167[A]:A:N3	3:a:167[A]:A:H2'	2.23	0.54
1:O:11:LYS:HE3	2:T:168[A]:A:H61	1.73	0.54
2:bb:167[A]:A:H2'	2:bb:168[A]:A:H5'	1.90	0.54
1:E:95:ARG:HD3	1:E:108[B]:GLU:CD	2.33	0.53
4:ll:187[A]:U:H2'	4:ll:188[A]:U:H4'	1.88	0.53
1:J:72:SER:OG	1:L:104:ASP:O	2.22	0.53
4:qq:188:U:O5'	8:qq:202:HOH:O	2.19	0.53
1:D:40:ALA:HB2	4:h:188[A]:U:H5''	1.90	0.53
1:G:14:GLY:HA2	1:G:15:ASP:OD1	2.09	0.53
4:kk:188[A]:U:C2'	4:kk:189:U:H5'	2.38	0.52
2:bb:163[A]:A:C2	4:qq:188:U:O4	2.63	0.52
1:JJ:91:TYR:N	6:JJ:303:CL:CL	2.79	0.51
1:K:79[B]:ARG:NH2	3:Y:169:A:P	2.81	0.51
1:KK:57:VAL:HG21	1:KK:134:THR:HB	1.92	0.51
1:II:17:SER:N	8:II:303:HOH:O	2.42	0.51
1:K:106:THR:OG1	1:O:66:ARG:NH2	2.39	0.51
4:h:186[A]:U:O2'	4:h:187[A]:U:OP1	2.28	0.51
4:qq:185[A]:U:O2	4:qq:185[A]:U:O5'	2.29	0.51
1:A:106:THR:OG1	1:E:66:ARG:NH2	2.35	0.51
2:bb:165[A]:A:N3	8:bb:202:HOH:O	2.33	0.50
4:e:180:U:C1'	4:e:181[A]:U:OP1	2.59	0.50
2:V:162:A:O2'	2:V:163:A:O5'	2.28	0.50
1:E:30:LYS:NZ	1:G:121:SER:O	2.41	0.49
1:KK:40:ALA:HB2	4:qq:187[A]:U:C4'	2.42	0.49
3:Y:165[A]:A:H2	4:n:184[A]:U:H3	1.60	0.49
1:JJ:95:ARG:HD3	6:JJ:302:CL:CL	2.49	0.49
1:II:81:TRP:CD1	1:II:121:SER:HB3	2.48	0.49
4:kk:188[A]:U:C3'	4:kk:189:U:H5'	2.43	0.49
1:A:39[B]:ARG:HG2	1:A:41:ILE:CD1	2.42	0.49
1:JJ:47:VAL:HG12	1:JJ:48:GLN:N	2.28	0.49
1:B:57:VAL:HG22	1:B:140:VAL:HG22	1.95	0.49
1:E:82:THR:O	1:E:119:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:162:A:H2'	2:V:163:A:C8	2.47	0.48
4:qq:187[A]:U:O2'	4:qq:188:U:C5'	2.60	0.48
1:H:110:GLU:OE1	6:H:202:CL:CL	2.67	0.48
4:i:184[A]:U:C2'	4:i:185[A]:U:OP1	2.61	0.48
4:h:185[A]:U:C2'	4:h:186[A]:U:H5'	2.44	0.48
1:KK:40:ALA:CB	4:qq:187[A]:U:H4'	2.41	0.48
1:O:14:GLY:HA2	4:i:184[A]:U:C4'	2.44	0.48
6:II:202:CL:CL	8:II:306:HOH:O	2.57	0.48
1:B:19:VAL:HG22	1:B:20:VAL:H	1.78	0.48
1:E:95:ARG:HD3	1:E:108[B]:GLU:CG	2.44	0.48
1:M:23:ILE:O	1:M:25:ALA:N	2.45	0.48
1:KK:70:PHE:CD1	1:KK:158:PHE:HB3	2.49	0.48
1:HH:100:PHE:CD2	1:HH:130[B]:LEU:HD21	2.49	0.48
1:B:81:TRP:O	1:B:151:ALA:N	2.43	0.48
1:F:116:ILE:HD11	1:J:117:ASN:OD1	2.14	0.48
1:B:37:TRP:HH2	1:B:66:ARG:HD2	1.79	0.47
1:G:128:THR:HG23	1:HH:15:ASP:CB	2.44	0.47
1:II:37:TRP:HH2	1:II:66:ARG:HD2	1.79	0.47
1:D:33:PRO:CD	6:JJ:302:CL:CL	2.99	0.47
2:bb:163[A]:A:OP2	2:bb:163[A]:A:C8	2.67	0.47
1:C:117:ASN:OD1	1:D:116:ILE:HD11	2.14	0.47
1:G:44:GLU:OE2	1:H:112:ARG:NH2	2.39	0.47
1:K:79[B]:ARG:HH22	3:Y:169:A:P	2.36	0.47
1:C:44:GLU:OE2	1:D:112:ARG:NH2	2.46	0.47
4:e:185[A]:U:O2'	4:e:186[A]:U:C5'	2.63	0.47
4:e:185[A]:U:H1'	4:e:186[A]:U:OP1	2.15	0.46
1:G:14:GLY:HA2	1:G:15:ASP:HA	1.57	0.46
1:JJ:47:VAL:HG12	1:JJ:48:GLN:H	1.80	0.46
1:KK:73:VAL:HG22	1:KK:156:CYS:HB2	1.97	0.46
1:JJ:18[A]:ASN:O	8:JJ:404:HOH:O	2.21	0.46
2:bb:167[A]:A:H2'	2:bb:168[A]:A:C5'	2.46	0.46
2:P:165[A]:A:C2	2:P:166[A]:A:C5	3.03	0.46
1:H:81:TRP:O	1:H:151:ALA:N	2.47	0.46
1:J:79:ARG:NH2	4:n:187[A]:U:OP1	2.49	0.46
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.51	0.46
1:F:152:LEU:O	6:F:201:CL:CL	2.70	0.46
1:N:85:THR:HG22	1:O:116:ILE:HG21	1.98	0.46
1:L:48:GLN:HB2	1:L:51:ILE:HG22	1.97	0.45
1:II:117:ASN:O	1:JJ:115:ASN:HA	2.15	0.45
1:C:44:GLU:OE2	1:D:112:ARG:NH1	2.47	0.45
1:G:99:LEU:HD11	1:G:142:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:TRP:O	1:L:151:ALA:N	2.41	0.45
1:KK:73:VAL:CG2	1:KK:156:CYS:HB2	2.46	0.45
1:E:95:ARG:HD3	1:E:108[B]:GLU:HG2	1.99	0.45
1:O:13:THR:O	1:O:13:THR:OG1	2.30	0.45
1:O:16:ASN:O	1:O:16:ASN:ND2	2.50	0.45
1:O:14:GLY:HA3	4:i:184[A]:U:C5'	2.47	0.45
1:KK:115:ASN:OD1	1:KK:117:ASN:N	2.47	0.45
3:TT:164[A]:A:C8	3:TT:164[A]:A:H5''	2.52	0.45
2:bb:161[A]:A:N3	8:bb:203:HOH:O	2.36	0.45
1:G:125:ARG:NH2	4:WW:170:U:H5''	2.32	0.45
2:S:162:A:H1'	2:S:163[A]:A:N7	2.32	0.45
1:B:37:TRP:CE2	1:B:39:ARG:HD3	2.52	0.45
1:C:152:LEU:O	6:C:206:CL:CL	2.72	0.45
1:K:155:SER:OG	3:Y:168[A]:A:OP1	2.30	0.45
1:A:117:ASN:O	1:B:115:ASN:HA	2.17	0.44
1:G:99:LEU:HD13	1:G:139[B]:ASN:ND2	2.32	0.44
1:K:148[B]:ARG:HG2	1:K:148[B]:ARG:NH1	2.28	0.44
4:i:187[A]:U:N3	4:i:188[A]:U:O4	2.49	0.44
4:WW:173:U:O2	4:WW:173:U:O4'	2.35	0.44
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.53	0.44
1:F:68:ASP:OD1	1:F:68:ASP:N	2.51	0.44
1:L:81:TRP:CD1	1:L:121:SER:HB3	2.53	0.44
1:A:38:VAL:HB	4:e:185[A]:U:H5	1.83	0.44
1:M:110:GLU:OE2	1:M:112:ARG:NE	2.50	0.44
1:I:66:ARG:NH2	1:J:106:THR:OG1	2.36	0.44
1:M:97:LYS:HA	1:M:107:GLU:O	2.17	0.44
1:J:33:PRO:O	1:K:65:PHE:HA	2.18	0.44
1:M:37:TRP:CE2	1:M:39:ARG:HD3	2.53	0.44
1:HH:100:PHE:CE2	1:HH:130[B]:LEU:HD21	2.53	0.44
1:KK:49:SER:N	6:KK:205:CL:CL	2.88	0.44
1:O:91:TYR:CE2	1:O:116:ILE:HG23	2.53	0.44
1:HH:97:LYS:HA	1:HH:107:GLU:O	2.18	0.44
4:kk:185[A]:U:O5'	4:kk:185[A]:U:H6	2.01	0.44
1:C:81:TRP:O	1:C:151:ALA:N	2.50	0.43
4:h:186[A]:U:HO2'	4:h:187[A]:U:P	2.41	0.43
1:A:115:ASN:OD1	1:A:117:ASN:N	2.50	0.43
1:N:122:VAL:HG22	1:N:123:GLY:H	1.83	0.43
3:TT:165:A:H5'	8:TT:301:HOH:O	2.18	0.43
3:TT:167[A]:A:C2	3:TT:168[A]:A:H1'	2.52	0.43
1:A:39[A]:ARG:NH2	1:O:33:PRO:O	2.51	0.43
1:L:11:LYS:HZ1	1:L:14:GLY:HA2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KK:70:PHE:CG	1:KK:158:PHE:HB3	2.53	0.43
6:H:202:CL:CL	1:HH:33:PRO:HD2	2.55	0.43
1:I:37:TRP:HH2	1:I:66:ARG:HD2	1.83	0.43
4:WW:167[A]:U:P	4:WW:167[A]:U:H3'	2.58	0.43
3:TT:165:A:C8	3:TT:165:A:OP2	2.71	0.43
1:L:38:VAL:HG23	3:a:165[A]:A:H1'	2.01	0.43
1:KK:57:VAL:HB	1:KK:135:VAL:O	2.18	0.43
1:L:7:LYS:HA	1:L:7:LYS:HD3	1.86	0.43
4:h:186[A]:U:O2'	4:h:187[A]:U:P	2.77	0.43
1:HH:57:VAL:HG22	1:HH:140:VAL:CG2	2.48	0.43
1:F:151:ALA:HB1	6:F:201:CL:CL	2.56	0.43
1:N:23:ILE:O	1:N:25:ALA:N	2.49	0.43
4:e:189[A]:U:H2'	4:e:190[A]:U:O4'	2.19	0.43
1:G:33:PRO:O	1:HH:39:ARG:NH2	2.52	0.43
1:B:30:LYS:HB2	1:N:22[B]:MET:SD	2.59	0.42
1:D:81:TRP:CD1	1:D:121:SER:HB3	2.54	0.42
1:H:110:GLU:HB2	6:H:202:CL:CL	2.56	0.42
1:C:57:VAL:HG22	1:C:140[A]:VAL:HG22	2.01	0.42
1:G:81:TRP:CD1	1:G:121:SER:HB3	2.55	0.42
1:II:44:GLU:OE2	6:II:203:CL:CL	2.74	0.42
1:L:11:LYS:O	1:L:11:LYS:HG2	2.18	0.42
1:G:128:THR:HG23	1:HH:15:ASP:HB3	2.01	0.42
1:M:80:ALA:O	1:M:121:SER:HA	2.20	0.42
3:a:165[A]:A:C5	3:a:166[A]:A:N7	2.88	0.42
5:m:188[A]:U:O2	5:m:188[A]:U:H2'	2.20	0.42
1:A:30:LYS:HG3	1:J:24:ARG:HA	2.01	0.42
1:I:117:ASN:O	1:J:115:ASN:HA	2.20	0.42
3:Y:167[A]:A:C2'	3:Y:168[A]:A:O5'	2.68	0.42
1:J:40:ALA:CB	4:n:186[A]:U:H5''	2.50	0.42
1:C:118[A]:THR:HA	1:D:114:SER:O	2.20	0.42
1:D:18:ASN:CA	1:II:129:ASN:HD21	2.33	0.42
1:N:81:TRP:O	1:N:151:ALA:N	2.51	0.42
1:O:11:LYS:HE3	2:T:168[A]:A:N6	2.33	0.42
1:G:73:VAL:HG22	1:G:156:CYS:HB2	2.01	0.42
1:L:76[B]:MET:SD	1:L:157:CYS:SG	3.18	0.42
1:O:11:LYS:O	1:O:12:SER:HB2	2.20	0.42
1:D:40:ALA:CB	4:h:188[A]:U:H5''	2.50	0.41
1:H:95:ARG:CD	6:H:202:CL:CL	3.04	0.41
1:JJ:45:VAL:HB	1:JJ:53:PHE:CE2	2.55	0.41
1:B:73:VAL:HG22	1:B:156:CYS:HB2	2.02	0.41
1:D:144:ARG:NE	6:D:201:CL:CL	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:PRO:O	1:F:39:ARG:NH2	2.53	0.41
1:F:117:ASN:HB3	1:G:116:ILE:HG12	2.02	0.41
1:I:24:ARG:HA	1:L:30:LYS:HG3	2.01	0.41
1:C:117:ASN:O	1:D:115:ASN:HA	2.20	0.41
1:F:81:TRP:CD1	1:F:121:SER:HB3	2.55	0.41
1:L:13:THR:O	1:L:13:THR:OG1	2.36	0.41
1:M:85:THR:HG22	1:N:116:ILE:HG21	2.02	0.41
2:bb:163[A]:A:H8	2:bb:163[A]:A:O5'	2.03	0.41
1:F:47[B]:VAL:HG23	1:F:147:CYS:O	2.20	0.41
2:T:164[A]:A:H4'	1:HH:17:SER:HA	2.02	0.41
3:TT:164[A]:A:C8	3:TT:164[A]:A:C5'	3.03	0.41
1:C:151:ALA:HB1	6:C:206:CL:CL	2.57	0.41
1:F:24:ARG:HA	1:II:30:LYS:HG3	2.03	0.41
1:H:57:VAL:HG22	1:H:140:VAL:HG22	2.03	0.41
2:bb:164[A]:A:N1	4:qq:187[A]:U:O4	2.53	0.41
1:A:88:VAL:O	1:A:89:ASN:HB2	2.20	0.41
3:Y:167[A]:A:O2'	3:Y:168[A]:A:O5'	2.34	0.41
1:H:142:GLU:OE1	6:H:201:CL:CL	2.76	0.41
1:A:47:VAL:CG1	1:A:147:CYS:O	2.68	0.41
1:J:17:SER:HB3	2:P:164[A]:A:O3'	2.20	0.41
1:K:38:VAL:HG23	4:n:184[A]:U:H1'	2.03	0.41
3:a:167[A]:A:C2	3:a:168[A]:A:C8	3.08	0.41
1:A:131:ARG:O	1:K:129:ASN:ND2	2.43	0.41
1:B:50:GLY:N	8:B:403:HOH:O	2.39	0.41
1:F:16:ASN:O	1:F:17:SER:HB2	2.21	0.41
1:J:39:ARG:NH2	1:K:33:PRO:O	2.54	0.41
1:L:8:PRO:O	6:L:501:CL:CL	2.76	0.41
1:M:91:TYR:CE1	1:M:116:ILE:HG23	2.56	0.41
1:O:11:LYS:NZ	1:O:11:LYS:HB3	2.36	0.41
2:T:166[A]:A:N1	4:i:184[A]:U:O4	2.54	0.41
4:e:185[A]:U:O2'	4:e:186[A]:U:H6	2.02	0.41
1:G:152:LEU:O	6:G:301:CL:CL	2.75	0.41
1:O:17:SER:HA	4:i:185[A]:U:OP1	2.20	0.41
1:JJ:37:TRP:HH2	1:JJ:66:ARG:HD2	1.86	0.41
1:JJ:127:PRO:HB2	1:JJ:129:ASN:OD1	2.21	0.41
1:J:29:PRO:HD3	1:K:81:TRP:CZ2	2.56	0.40
1:N:115:ASN:OD1	1:N:117:ASN:N	2.50	0.40
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.56	0.40
1:E:37:TRP:CE2	1:E:39:ARG:HD3	2.56	0.40
1:I:17:SER:OG	3:a:165[A]:A:O5'	2.39	0.40
1:M:38:VAL:HG22	1:M:157:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJ:108:GLU:HB3	6:JJ:302:CL:CL	2.59	0.40
1:E:21:THR:HG22	4:n:184[A]:U:H5'	2.02	0.40
1:F:114:SER:O	1:J:118:THR:HA	2.22	0.40
1:N:110:GLU:OE2	1:N:112:ARG:NE	2.46	0.40
1:B:52:ALA:HB2	1:B:144:ARG:CZ	2.51	0.40
1:B:57:VAL:HG22	1:B:140:VAL:CG2	2.50	0.40
1:H:22[A]:MET:HG3	1:H:23:ILE:N	2.36	0.40
1:II:68:ASP:OD1	1:II:68:ASP:N	2.54	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:308:HOH:O	8:N:202:HOH:O[6_566]	1.91	0.29
4:II:186[A]:U:OP1	8:II:305:HOH:O[6_566]	1.91	0.29
2:S:164[A]:A:O2'	8:KK:317:HOH:O[12_665]	1.97	0.23
6:TT:201:CL:CL	8:B:420:HOH:O[6_566]	2.07	0.13
1:H:15:ASP:N	4:e:183[A]:U:OP2[6_566]	2.08	0.12
1:A:15:ASP:N	2:X:164[A]:A:OP1[12_665]	2.11	0.09
1:L:72:SER:OG	1:N:104:ASP:O[6_566]	2.14	0.06
1:L:26:GLY:O	1:M:81:TRP:HE1[6_566]	1.57	0.03
2:bb:164[A]:A:O2'	8:JJ:425:HOH:O[12_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/159 (93%)	138 (93%)	9 (6%)	1 (1%)	18	40
1	B	143/159 (90%)	134 (94%)	8 (6%)	1 (1%)	18	40
1	C	143/159 (90%)	135 (94%)	8 (6%)	0	100	100
1	D	148/159 (93%)	140 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	147/159 (92%)	138 (94%)	9 (6%)	0	100	100
1	F	152/159 (96%)	143 (94%)	8 (5%)	1 (1%)	18	40
1	G	150/159 (94%)	142 (95%)	8 (5%)	0	100	100
1	GG	146/159 (92%)	139 (95%)	7 (5%)	0	100	100
1	H	147/159 (92%)	136 (92%)	11 (8%)	0	100	100
1	HH	150/159 (94%)	144 (96%)	6 (4%)	0	100	100
1	I	145/159 (91%)	139 (96%)	6 (4%)	0	100	100
1	II	149/159 (94%)	139 (93%)	10 (7%)	0	100	100
1	J	152/159 (96%)	143 (94%)	8 (5%)	1 (1%)	18	40
1	JJ	142/159 (89%)	135 (95%)	7 (5%)	0	100	100
1	K	156/159 (98%)	147 (94%)	9 (6%)	0	100	100
1	KK	143/159 (90%)	136 (95%)	7 (5%)	0	100	100
1	L	170/159 (107%)	146 (86%)	17 (10%)	7 (4%)	2	5
1	M	155/159 (98%)	145 (94%)	9 (6%)	1 (1%)	21	45
1	N	155/159 (98%)	141 (91%)	13 (8%)	1 (1%)	21	45
1	O	150/159 (94%)	138 (92%)	11 (7%)	1 (1%)	18	40
All	All	2991/3180 (94%)	2798 (94%)	179 (6%)	14 (0%)	24	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	15	ASP
1	L	7	LYS
1	L	8	PRO
1	L	10	ARG
1	M	122	VAL
1	N	122	VAL
1	O	12	SER
1	L	13	THR
1	A	17	SER
1	F	17	SER
1	L	6	VAL
1	L	9	ASN
1	B	37	TRP
1	L	14	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/140 (96%)	134 (100%)	0	100	100
1	B	129/140 (92%)	128 (99%)	1 (1%)	73	84
1	C	129/140 (92%)	127 (98%)	2 (2%)	55	74
1	D	134/140 (96%)	134 (100%)	0	100	100
1	E	133/140 (95%)	133 (100%)	0	100	100
1	F	138/140 (99%)	138 (100%)	0	100	100
1	G	135/140 (96%)	135 (100%)	0	100	100
1	GG	132/140 (94%)	132 (100%)	0	100	100
1	H	133/140 (95%)	133 (100%)	0	100	100
1	HH	136/140 (97%)	136 (100%)	0	100	100
1	I	131/140 (94%)	131 (100%)	0	100	100
1	II	135/140 (96%)	135 (100%)	0	100	100
1	J	137/140 (98%)	137 (100%)	0	100	100
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	142/140 (101%)	142 (100%)	0	100	100
1	KK	129/140 (92%)	128 (99%)	1 (1%)	73	84
1	L	154/140 (110%)	154 (100%)	0	100	100
1	M	141/140 (101%)	139 (99%)	2 (1%)	59	76
1	N	141/140 (101%)	141 (100%)	0	100	100
1	O	135/140 (96%)	135 (100%)	0	100	100
All	All	2706/2800 (97%)	2700 (100%)	6 (0%)	87	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	THR
1	C	24	ARG
1	C	106	THR

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Mol	Chain	Res	Type
1	M	38	VAL
1	M	122	VAL
1	KK	155[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	C	117	ASN
1	D	18	ASN
1	E	117	ASN
1	F	89	ASN
1	F	117	ASN
1	I	117	ASN
1	K	117	ASN
1	N	117	ASN
1	O	16	ASN
1	O	18[A]	ASN
1	O	89	ASN
1	HH	18	ASN
1	HH	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	6/12 (50%)	1 (16%)	0
2	S	6/12 (50%)	1 (16%)	0
2	T	4/12 (33%)	1 (25%)	0
2	UU	6/12 (50%)	1 (16%)	0
2	V	7/12 (58%)	2 (28%)	0
2	X	7/12 (58%)	0	0
2	bb	10/12 (83%)	5 (50%)	0
3	TT	5/11 (45%)	3 (60%)	1 (20%)
3	Y	8/11 (72%)	4 (50%)	0
3	a	4/11 (36%)	2 (50%)	0
4	WW	9/13 (69%)	5 (55%)	1 (11%)
4	e	10/13 (76%)	5 (50%)	0
4	h	6/13 (46%)	2 (33%)	0
4	i	4/13 (30%)	1 (25%)	0
4	kk	5/13 (38%)	3 (60%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	ll	4/13 (30%)	0	0
4	n	6/13 (46%)	0	0
4	qq	5/13 (38%)	3 (60%)	0
5	m	8/11 (72%)	3 (37%)	0
All	All	120/232 (51%)	42 (35%)	2 (1%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	P	164[A]	A
2	S	163[A]	A
2	T	168[A]	A
2	V	163	A
2	V	169[A]	A
3	Y	168[A]	A
3	Y	169	A
3	Y	170	A
3	Y	171	A
3	a	165[A]	A
3	a	168[A]	A
4	e	181[A]	U
4	e	183[A]	U
4	e	184[A]	U
4	e	185[A]	U
4	e	186[A]	U
4	h	186[A]	U
4	h	187[A]	U
4	i	185[A]	U
5	m	183[A]	U
5	m	188[A]	U
5	m	189[A]	U
3	TT	165	A
3	TT	166[A]	A
3	TT	168[A]	A
2	UU	164[A]	A
4	WW	167[A]	U
4	WW	169	U
4	WW	172	U
4	WW	173	U
4	WW	174	U
2	bb	159	A
2	bb	160	A

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Mol	Chain	Res	Type
2	bb	161[A]	A
2	bb	163[A]	A
2	bb	168[A]	A
4	kk	185[A]	U
4	kk	188[A]	U
4	kk	189	U
4	qq	186[A]	U
4	qq	187[A]	U
4	qq	188	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	TT	164[A]	A
4	WW	173	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 53 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	145/159 (91%)	0.59	8 (5%)	30	25	34, 55, 84, 161	4 (2%)
1	B	143/159 (89%)	0.49	7 (4%)	35	28	29, 52, 76, 101	2 (1%)
1	C	142/159 (89%)	0.24	4 (2%)	55	46	32, 44, 61, 98	4 (2%)
1	D	144/159 (90%)	0.20	5 (3%)	47	39	27, 40, 65, 122	4 (2%)
1	E	144/159 (90%)	0.38	5 (3%)	47	39	34, 44, 76, 129	4 (2%)
1	F	144/159 (90%)	0.61	6 (4%)	40	32	31, 56, 82, 140	6 (4%)
1	G	146/159 (91%)	0.48	9 (6%)	26	22	34, 48, 84, 167	3 (2%)
1	GG	145/159 (91%)	0.13	3 (2%)	63	54	26, 35, 64, 211	2 (1%)
1	H	145/159 (91%)	0.40	6 (4%)	41	33	31, 49, 73, 195	2 (1%)
1	HH	145/159 (91%)	0.35	4 (2%)	55	46	23, 39, 68, 119	4 (2%)
1	I	144/159 (90%)	0.76	10 (6%)	23	19	29, 62, 79, 125	4 (2%)
1	II	143/159 (89%)	0.34	5 (3%)	47	39	23, 41, 61, 99	3 (2%)
1	J	147/159 (92%)	0.96	13 (8%)	15	14	39, 67, 96, 162	8 (5%)
1	JJ	144/159 (90%)	0.13	3 (2%)	63	54	23, 34, 60, 135	2 (1%)
1	K	145/159 (91%)	0.91	12 (8%)	17	15	31, 67, 88, 153	10 (6%)
1	KK	144/159 (90%)	0.09	0	100	100	22, 33, 60, 120	3 (2%)
1	L	157/159 (98%)	1.49	37 (23%)	2	2	41, 79, 123, 150	11 (7%)
1	M	144/159 (90%)	1.51	31 (21%)	2	2	40, 81, 108, 137	11 (7%)
1	N	144/159 (90%)	1.12	17 (11%)	9	9	32, 75, 121, 154	9 (6%)
1	O	150/159 (94%)	0.89	10 (6%)	24	21	30, 67, 116, 158	7 (4%)
2	P	7/12 (58%)	3.02	7 (100%)	0	0	74, 86, 134, 140	6 (85%)
2	S	7/12 (58%)	2.42	4 (57%)	0	0	55, 77, 121, 166	5 (71%)
2	T	5/12 (41%)	1.83	1 (20%)	3	3	58, 59, 76, 83	4 (80%)
2	UU	7/12 (58%)	2.86	6 (85%)	0	0	45, 58, 74, 75	7 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	V	8/12 (66%)	2.52	4 (50%) 0 0	64, 94, 152, 180	4 (50%)
2	X	8/12 (66%)	3.68	8 (100%) 0 0	59, 78, 102, 110	8 (100%)
2	bb	11/12 (91%)	4.13	9 (81%) 0 0	65, 73, 80, 85	8 (72%)
3	TT	6/11 (54%)	4.01	5 (83%) 0 0	63, 135, 164, 245	1 (16%)
3	Y	9/11 (81%)	3.64	9 (100%) 0 0	59, 64, 86, 96	9 (100%)
3	a	5/11 (45%)	6.53	5 (100%) 0 0	55, 73, 84, 142	4 (80%)
4	WW	10/13 (76%)	3.41	10 (100%) 0 0	83, 124, 134, 138	6 (60%)
4	e	11/13 (84%)	3.80	11 (100%) 0 0	76, 94, 118, 120	11 (100%)
4	h	7/13 (53%)	3.07	6 (85%) 0 0	52, 67, 82, 91	7 (100%)
4	i	5/13 (38%)	3.28	5 (100%) 0 0	63, 70, 93, 97	3 (60%)
4	kk	6/13 (46%)	4.46	6 (100%) 0 0	74, 84, 101, 120	6 (100%)
4	ll	5/13 (38%)	1.96	2 (40%) 1 0	54, 62, 69, 71	3 (60%)
4	n	7/13 (53%)	3.11	6 (85%) 0 0	65, 71, 84, 102	7 (100%)
4	qq	6/13 (46%)	2.42	3 (50%) 0 0	55, 83, 128, 156	1 (16%)
5	m	9/11 (81%)	3.36	9 (100%) 0 0	69, 81, 103, 106	9 (100%)
All	All	3044/3412 (89%)	0.73	311 (10%) 12 11	22, 54, 98, 245	212 (6%)

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	a	164[A]	A	8.9
3	a	168[A]	A	7.7
2	bb	160	A	6.8
4	kk	188[A]	U	6.4
1	L	6	VAL	6.3
3	a	165[A]	A	6.1
1	L	8	PRO	5.9
2	bb	158	A	5.8
1	E	108[A]	GLU	5.8
3	a	167[A]	A	5.8
1	L	7	LYS	5.8
3	TT	168[A]	A	5.7
4	i	188[A]	U	5.7
4	qq	188	U	5.6
4	n	188[A]	U	5.6
1	GG	15	ASP	5.3
1	II	92[A]	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	X	169[A]	A	5.2
2	bb	161[A]	A	5.2
2	bb	162[A]	A	5.1
2	bb	159	A	5.1
4	kk	189	U	5.1
2	bb	168[A]	A	4.9
1	G	14	GLY	4.8
3	TT	165	A	4.8
4	h	184[A]	U	4.7
5	m	188[A]	U	4.7
1	F	16	ASN	4.7
4	e	190[A]	U	4.7
1	M	121	SER	4.6
4	e	189[A]	U	4.6
4	WW	166[A]	U	4.6
5	m	189[A]	U	4.5
3	Y	168[A]	A	4.5
1	G	15	ASP	4.5
4	e	186[A]	U	4.5
1	K	24	ARG	4.4
4	e	188[A]	U	4.4
4	e	180	U	4.4
3	Y	170	A	4.4
4	ll	188[A]	U	4.4
2	X	162[A]	A	4.3
3	TT	164[A]	A	4.3
1	A	16	ASN	4.3
3	a	166[A]	A	4.3
1	L	10	ARG	4.3
2	V	169[A]	A	4.2
1	N	16	ASN	4.2
4	h	190[A]	U	4.2
4	kk	186[A]	U	4.2
3	TT	166[A]	A	4.2
1	O	24	ARG	4.2
4	i	184[A]	U	4.2
2	P	163[A]	A	4.1
2	S	163[A]	A	4.1
1	F	17	SER	4.1
1	L	4	GLY	4.1
4	e	181[A]	U	4.1
3	Y	167[A]	A	4.0

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Mol	Chain	Res	Type	RSRZ
3	Y	171	A	4.0
1	N	125	ARG	4.0
4	e	187[A]	U	4.0
4	e	182[A]	U	4.0
1	J	13	THR	4.0
2	UU	167[A]	A	4.0
4	kk	187[A]	U	4.0
1	L	9	ASN	4.0
2	bb	163[A]	A	4.0
4	n	187[A]	U	3.9
1	HH	27[A]	SER	3.9
4	WW	170	U	3.9
2	X	168[A]	A	3.9
1	H	16	ASN	3.9
2	X	166[A]	A	3.8
1	L	13	THR	3.8
4	WW	173	U	3.8
3	Y	166[A]	A	3.8
4	WW	165	U	3.7
4	h	189[A]	U	3.7
4	WW	171	U	3.7
4	kk	185[A]	U	3.7
2	V	168[A]	A	3.7
1	F	24	ARG	3.7
1	B	36	THR	3.7
2	UU	162[A]	A	3.7
1	J	14	GLY	3.7
4	n	182[A]	U	3.7
2	X	163[A]	A	3.6
1	L	5	LYS	3.6
4	WW	172	U	3.6
1	H	15	ASP	3.6
4	qq	187[A]	U	3.6
1	O	16	ASN	3.6
3	Y	169	A	3.6
1	M	24	ARG	3.5
1	G	16	ASN	3.5
1	L	120	ALA	3.5
5	m	190[A]	U	3.5
1	L	18[A]	ASN	3.5
1	M	18	ASN	3.5
1	L	50	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	X	165[A]	A	3.4
1	O	88[A]	VAL	3.4
4	WW	167[A]	U	3.4
4	kk	184[A]	U	3.4
5	m	182[A]	U	3.4
3	Y	163[A]	A	3.4
1	GG	16	ASN	3.4
1	O	13	THR	3.4
2	P	164[A]	A	3.4
1	HH	16	ASN	3.3
1	HH	24	ARG	3.3
1	M	16	ASN	3.3
1	J	108[A]	GLU	3.3
1	G	24	ARG	3.3
1	HH	15	ASP	3.3
1	JJ	16	ASN	3.3
2	P	169[A]	A	3.3
2	bb	167[A]	A	3.3
1	A	18[A]	ASN	3.3
1	B	21	THR	3.3
5	m	187[A]	U	3.2
1	L	40	ALA	3.2
1	K	111	GLY	3.2
1	E	16	ASN	3.2
1	E	24	ARG	3.2
1	G	48[A]	GLN	3.2
1	N	123	GLY	3.2
1	L	118	THR	3.2
2	P	168[A]	A	3.2
1	I	24	ARG	3.2
1	B	49[A]	SER	3.1
1	L	69	SER	3.1
1	L	16	ASN	3.1
1	G	139[A]	ASN	3.1
2	S	168[A]	A	3.1
2	UU	168[A]	A	3.1
1	I	47	VAL	3.1
3	TT	171	A	3.1
1	O	11	LYS	3.1
1	M	75	VAL	3.0
1	M	79[A]	ARG	3.0
2	T	168[A]	A	3.0

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Mol	Chain	Res	Type	RSRZ
2	UU	163[A]	A	3.0
1	M	150	VAL	3.0
5	m	185[A]	U	3.0
1	J	105	SER	3.0
1	L	12	SER	3.0
1	L	38	VAL	3.0
1	J	15	ASP	2.9
1	M	52	ALA	2.9
5	m	184[A]	U	2.9
1	J	16	ASN	2.9
1	M	38	VAL	2.9
4	e	183[A]	U	2.9
1	A	40	ALA	2.9
1	M	27[A]	SER	2.9
1	L	52	ALA	2.9
1	L	22[A]	MET	2.8
2	S	162	A	2.8
1	N	24	ARG	2.8
1	L	149[A]	GLN	2.8
1	M	91	TYR	2.8
1	L	25	ALA	2.8
1	M	137	ALA	2.8
5	m	183[A]	U	2.8
1	L	27[A]	SER	2.8
1	N	17	SER	2.8
1	L	11	LYS	2.8
2	V	163	A	2.8
3	Y	164[A]	A	2.8
1	M	95[A]	ARG	2.8
2	P	166[A]	A	2.7
4	WW	168	U	2.7
4	qq	183	U	2.7
1	L	15	ASP	2.7
1	I	48	GLN	2.7
2	X	164[A]	A	2.7
1	L	101[A]	LYS	2.7
1	N	145	SER	2.7
1	B	24	ARG	2.7
4	h	187[A]	U	2.7
1	M	20	VAL	2.7
1	B	17	SER	2.7
1	A	125	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	125	ARG	2.6
1	D	47[A]	VAL	2.6
4	h	188[A]	U	2.6
1	GG	17	SER	2.6
1	L	122	VAL	2.6
1	M	122	VAL	2.6
4	n	186[A]	U	2.6
4	WW	174	U	2.6
1	C	105[A]	SER	2.6
1	E	27[A]	SER	2.6
1	J	125	ARG	2.6
1	C	48[A]	GLN	2.6
1	G	25	ALA	2.6
1	D	24	ARG	2.5
4	n	183[A]	U	2.5
1	B	22[A]	MET	2.5
1	M	134	THR	2.5
1	D	16	ASN	2.5
1	K	15	ASP	2.5
1	E	148	ARG	2.5
1	H	24	ARG	2.5
1	L	68	ASP	2.5
1	L	121	SER	2.5
1	O	105[A]	SER	2.5
1	I	52	ALA	2.5
1	A	39[A]	ARG	2.5
2	S	167[A]	A	2.5
1	M	101	LYS	2.5
1	M	156	CYS	2.5
1	L	19[A]	VAL	2.5
1	I	68	ASP	2.4
1	L	24	ARG	2.4
1	II	24	ARG	2.4
2	V	162	A	2.4
1	J	38	VAL	2.4
1	L	55	VAL	2.4
1	M	72	SER	2.4
1	F	51	ILE	2.4
1	N	143	VAL	2.4
2	X	167[A]	A	2.4
2	UU	164[A]	A	2.4
2	UU	166[A]	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	92	SER	2.4
1	JJ	49[A]	SER	2.4
1	N	139	ASN	2.4
1	K	88	VAL	2.4
1	II	19[A]	VAL	2.4
1	H	27[A]	SER	2.4
4	i	187[A]	U	2.4
1	M	143[A]	VAL	2.3
1	M	157	CYS	2.3
1	I	27[A]	SER	2.3
1	N	49[A]	SER	2.3
1	II	17	SER	2.3
2	bb	166[A]	A	2.3
1	J	98	PRO	2.3
1	C	24	ARG	2.3
1	M	45	VAL	2.3
1	F	49[A]	SER	2.3
1	K	49[A]	SER	2.3
2	P	167[A]	A	2.3
1	K	148[A]	ARG	2.3
1	N	47	VAL	2.3
1	O	15	ASP	2.3
1	D	148	ARG	2.3
1	H	122	VAL	2.3
4	e	184[A]	U	2.3
1	I	16	ASN	2.3
1	I	23	ILE	2.3
1	M	26	GLY	2.3
1	II	26	GLY	2.3
1	L	3	ARG	2.2
1	N	88	VAL	2.2
1	H	123	GLY	2.2
1	K	16	ASN	2.2
3	Y	165[A]	A	2.2
1	K	134	THR	2.2
1	M	31	VAL	2.2
1	J	153	VAL	2.2
1	N	19[A]	VAL	2.2
1	N	38	VAL	2.2
1	L	26	GLY	2.2
1	L	114	SER	2.2
1	O	12	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	152	LEU	2.2
4	i	186[A]	U	2.2
4	n	185[A]	U	2.2
2	P	165[A]	A	2.2
1	G	17	SER	2.2
1	J	137	ALA	2.2
1	C	125	ARG	2.1
1	M	23	ILE	2.1
1	O	10	ARG	2.1
1	N	98	PRO	2.1
1	N	122	VAL	2.1
1	A	17	SER	2.1
1	A	49	SER	2.1
1	I	18[A]	ASN	2.1
1	D	22[A]	MET	2.1
4	h	185[A]	U	2.1
4	ll	184[A]	U	2.1
5	m	186[A]	U	2.1
1	N	79	ARG	2.1
1	I	157[A]	CYS	2.1
1	M	154	ILE	2.1
1	L	33	PRO	2.1
4	WW	169	U	2.1
1	K	116	ILE	2.1
1	M	151	ALA	2.1
1	K	149[A]	GLN	2.1
1	L	64	ASN	2.1
1	J	50	GLY	2.1
1	JJ	24	ARG	2.1
1	J	23	ILE	2.1
1	G	22[A]	MET	2.0
1	L	17	SER	2.0
1	M	139	ASN	2.0
1	M	74	THR	2.0
4	e	185[A]	U	2.0
4	i	185[A]	U	2.0
1	B	35	PRO	2.0
1	K	156	CYS	2.0
1	O	152	LEU	2.0
1	A	24	ARG	2.0
1	M	128[A]	THR	2.0
1	K	22[A]	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	L	501	1/1	0.62	0.26	111,111,111,111	0
6	CL	JJ	301	1/1	0.67	0.30	100,100,100,100	0
6	CL	JJ	303	1/1	0.72	0.22	52,52,52,52	0
6	CL	T	201	1/1	0.75	0.23	82,82,82,82	0
6	CL	B	301	1/1	0.77	0.20	68,68,68,68	0
6	CL	KK	203	1/1	0.77	0.26	86,86,86,86	0
7	MG	K	303	1/1	0.77	0.42	79,79,79,79	0
7	MG	E	201	1/1	0.78	0.32	71,71,71,71	0
6	CL	H	201	1/1	0.81	0.14	74,74,74,74	0
6	CL	C	204	1/1	0.81	0.23	91,91,91,91	0
6	CL	K	302	1/1	0.82	0.18	90,90,90,90	0
6	CL	KK	204	1/1	0.83	0.15	87,87,87,87	0
6	CL	TT	201	1/1	0.83	0.27	117,117,117,117	0
6	CL	C	202	1/1	0.83	0.19	74,74,74,74	0
7	MG	F	203	1/1	0.83	0.32	71,71,71,71	0
6	CL	H	202	1/1	0.83	0.32	88,88,88,88	0
6	CL	ll	201	1/1	0.84	0.12	78,78,78,78	0
6	CL	JJ	302	1/1	0.84	0.24	57,57,57,57	0
7	MG	HH	403	1/1	0.85	0.20	35,35,35,35	0
6	CL	B	302	1/1	0.86	0.23	82,82,82,82	0
6	CL	D	201	1/1	0.86	0.25	59,59,59,59	0
6	CL	C	201	1/1	0.87	0.22	51,51,51,51	0
6	CL	GG	201	1/1	0.87	0.37	82,82,82,82	0
6	CL	HH	401	1/1	0.87	0.36	68,68,68,68	0
6	CL	JJ	305	1/1	0.87	0.28	47,47,47,47	0
6	CL	HH	402	1/1	0.88	0.34	115,115,115,115	0
6	CL	C	203	1/1	0.89	0.12	57,57,57,57	0

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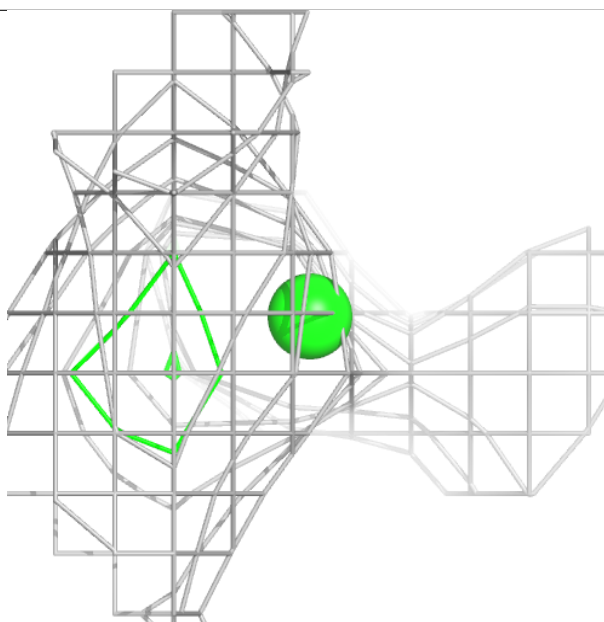
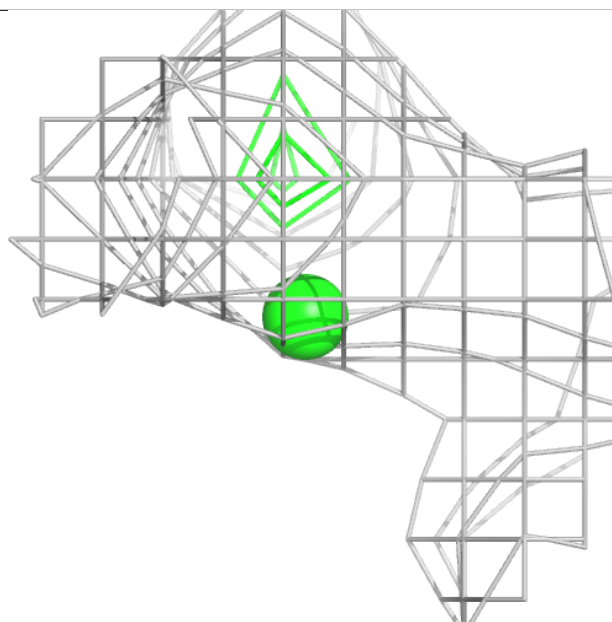
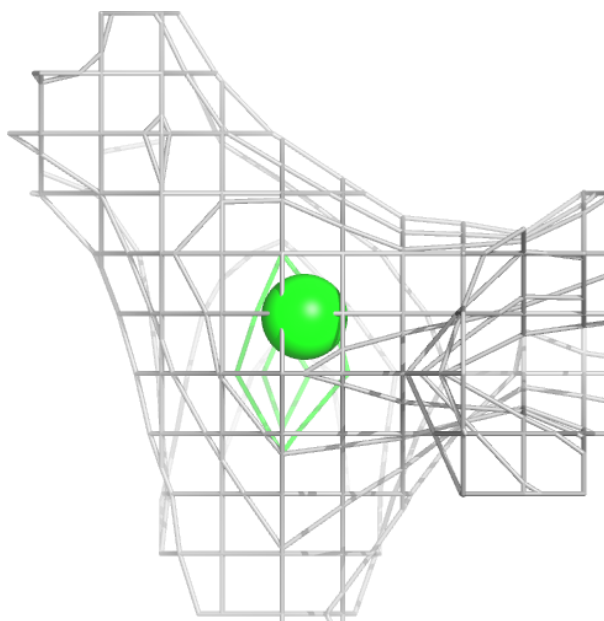
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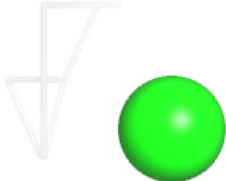
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	F	201	1/1	0.89	0.28	91,91,91,91	0
6	CL	K	301	1/1	0.89	0.24	45,45,45,45	0
6	CL	II	202	1/1	0.90	0.22	42,42,42,42	0
7	MG	E	202	1/1	0.90	0.20	39,39,39,39	0
6	CL	KK	205	1/1	0.90	0.10	72,72,72,72	0
7	MG	I	201	1/1	0.90	0.33	49,49,49,49	0
6	CL	KK	202	1/1	0.90	0.26	56,56,56,56	0
6	CL	G	301	1/1	0.90	0.27	104,104,104,104	0
6	CL	F	202	1/1	0.91	0.12	38,38,38,38	0
6	CL	II	203	1/1	0.91	0.24	93,93,93,93	0
7	MG	KK	206	1/1	0.91	0.09	25,25,25,25	0
7	MG	JJ	307	1/1	0.92	0.21	30,30,30,30	0
7	MG	GG	202	1/1	0.93	0.22	26,26,26,26	0
6	CL	D	202	1/1	0.93	0.23	71,71,71,71	0
6	CL	B	303	1/1	0.93	0.27	89,89,89,89	0
6	CL	JJ	304	1/1	0.93	0.19	83,83,83,83	0
7	MG	F	204	1/1	0.94	0.43	128,128,128,128	0
7	MG	G	303	1/1	0.94	0.14	43,43,43,43	0
6	CL	C	205	1/1	0.94	0.28	59,59,59,59	0
6	CL	II	201	1/1	0.94	0.17	66,66,66,66	0
6	CL	B	304	1/1	0.95	0.08	29,29,29,29	0
6	CL	G	302	1/1	0.95	0.10	59,59,59,59	0
6	CL	C	206	1/1	0.95	0.19	82,82,82,82	0
7	MG	HH	404	1/1	0.96	0.19	40,40,40,40	0
6	CL	KK	201	1/1	0.97	0.05	11,11,11,11	0
7	MG	JJ	306	1/1	0.97	0.23	149,149,149,149	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CL L 501:

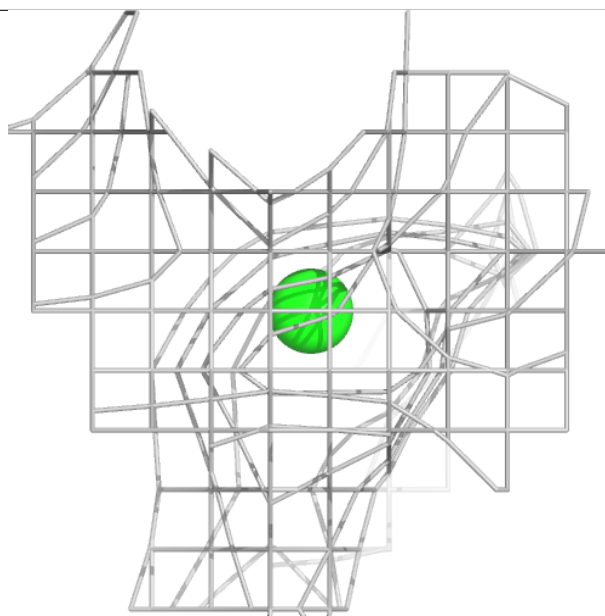
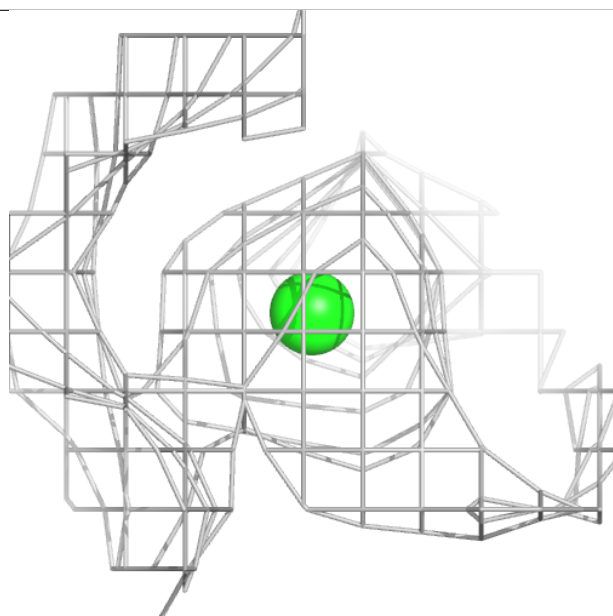
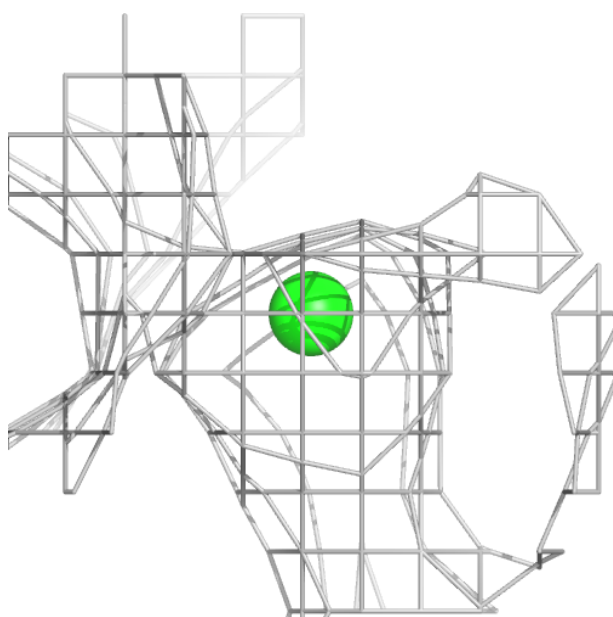
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL JJ 301: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

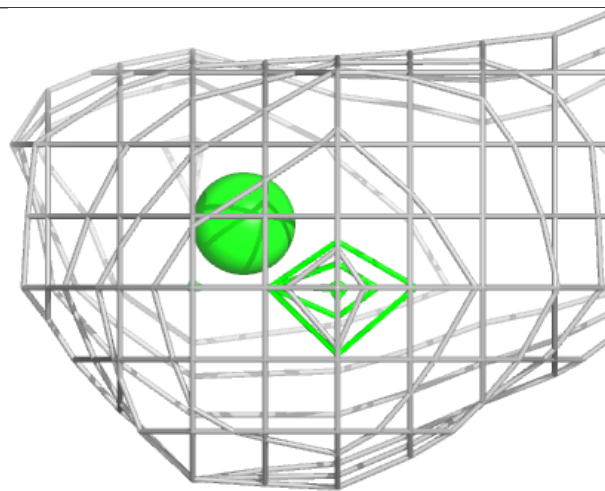
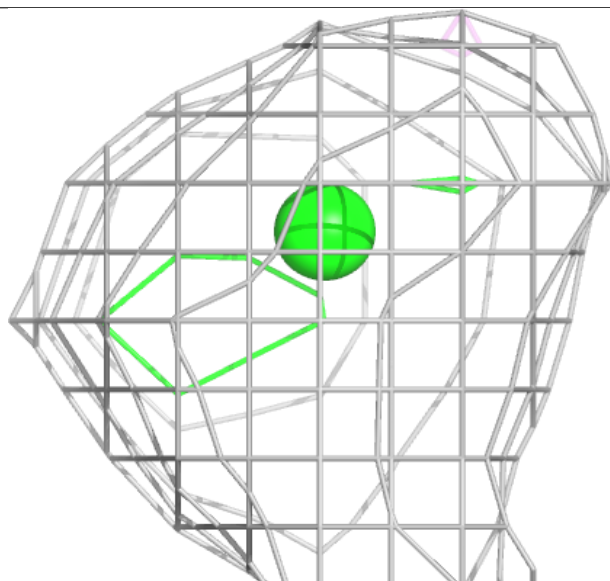
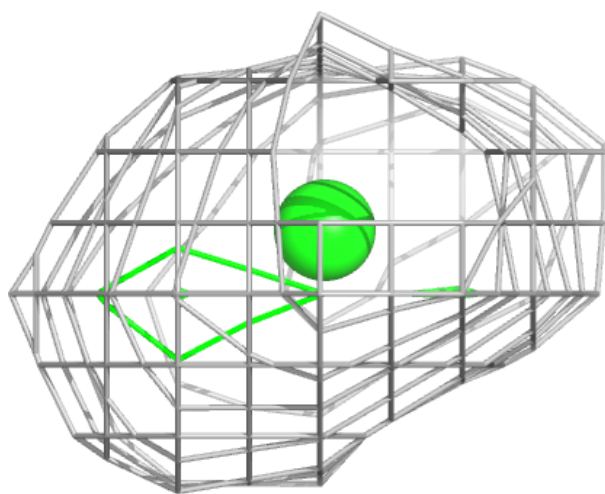
Electron density around CL JJ 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



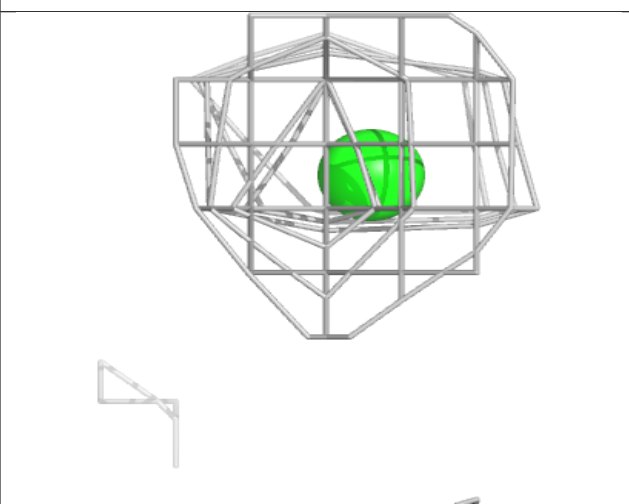
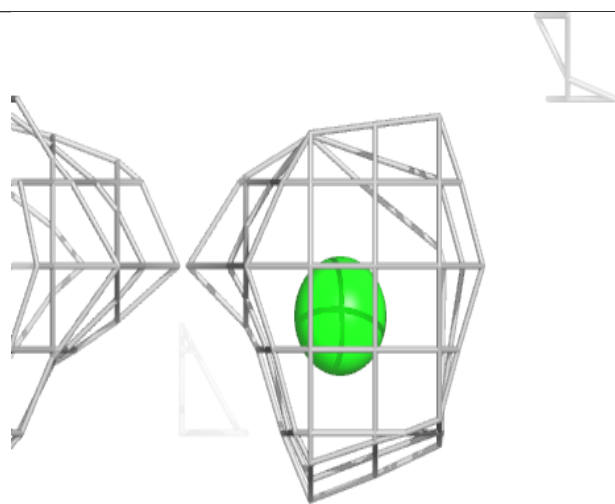
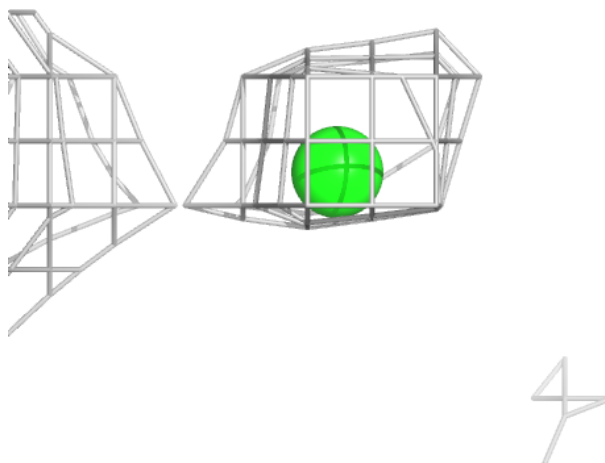
Electron density around CL T 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



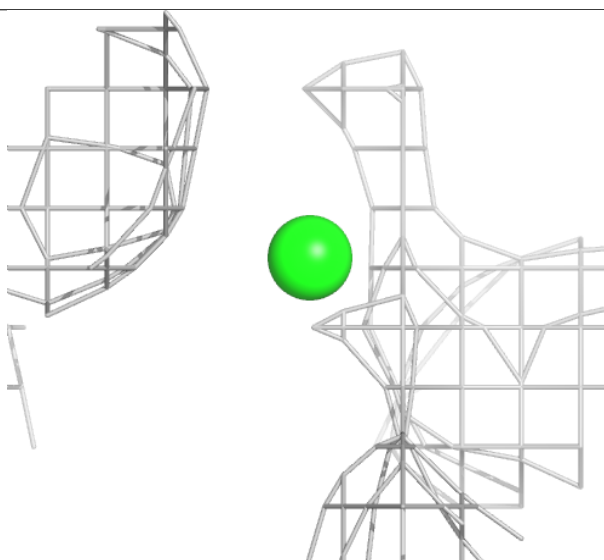
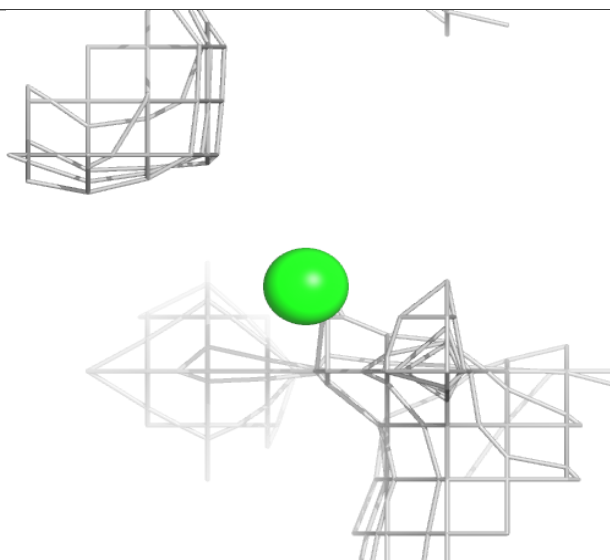
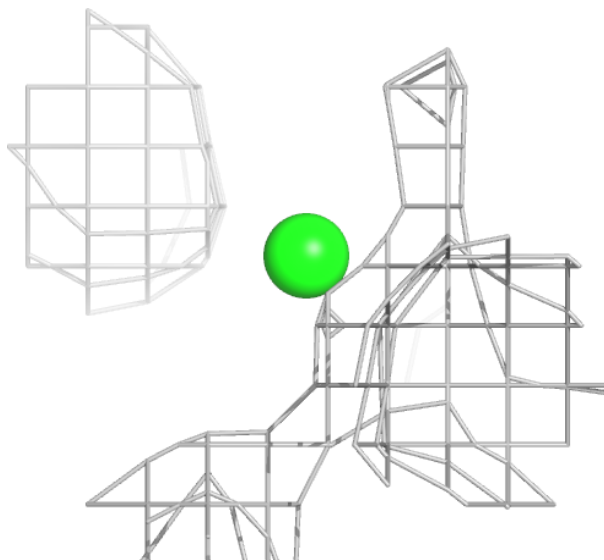
Electron density around CL B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



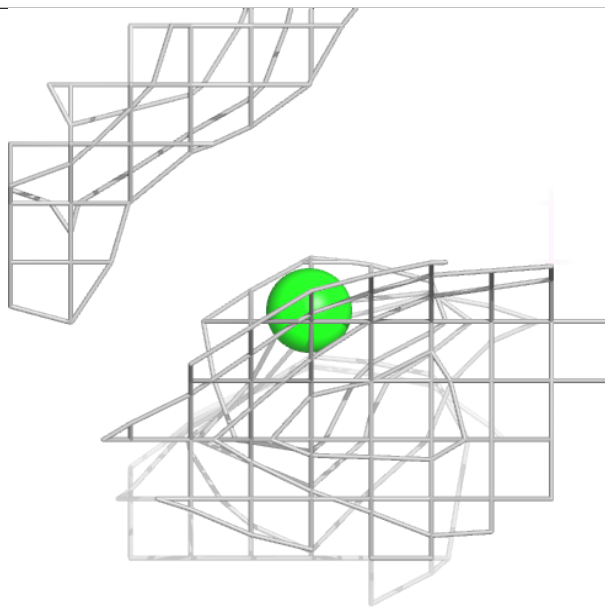
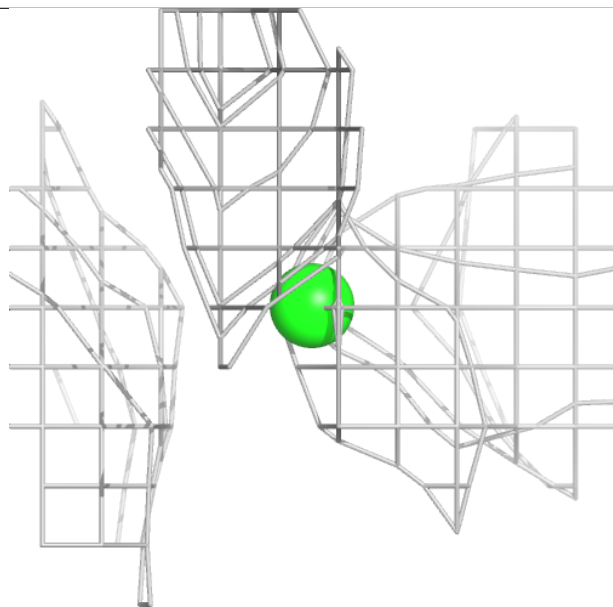
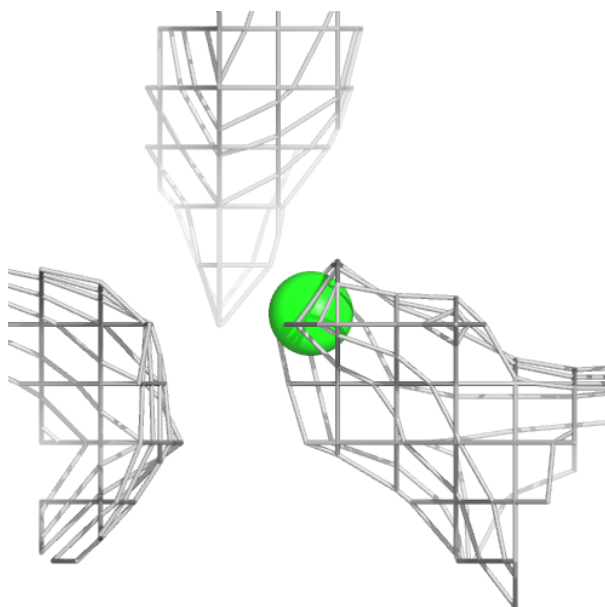
Electron density around CL KK 203:

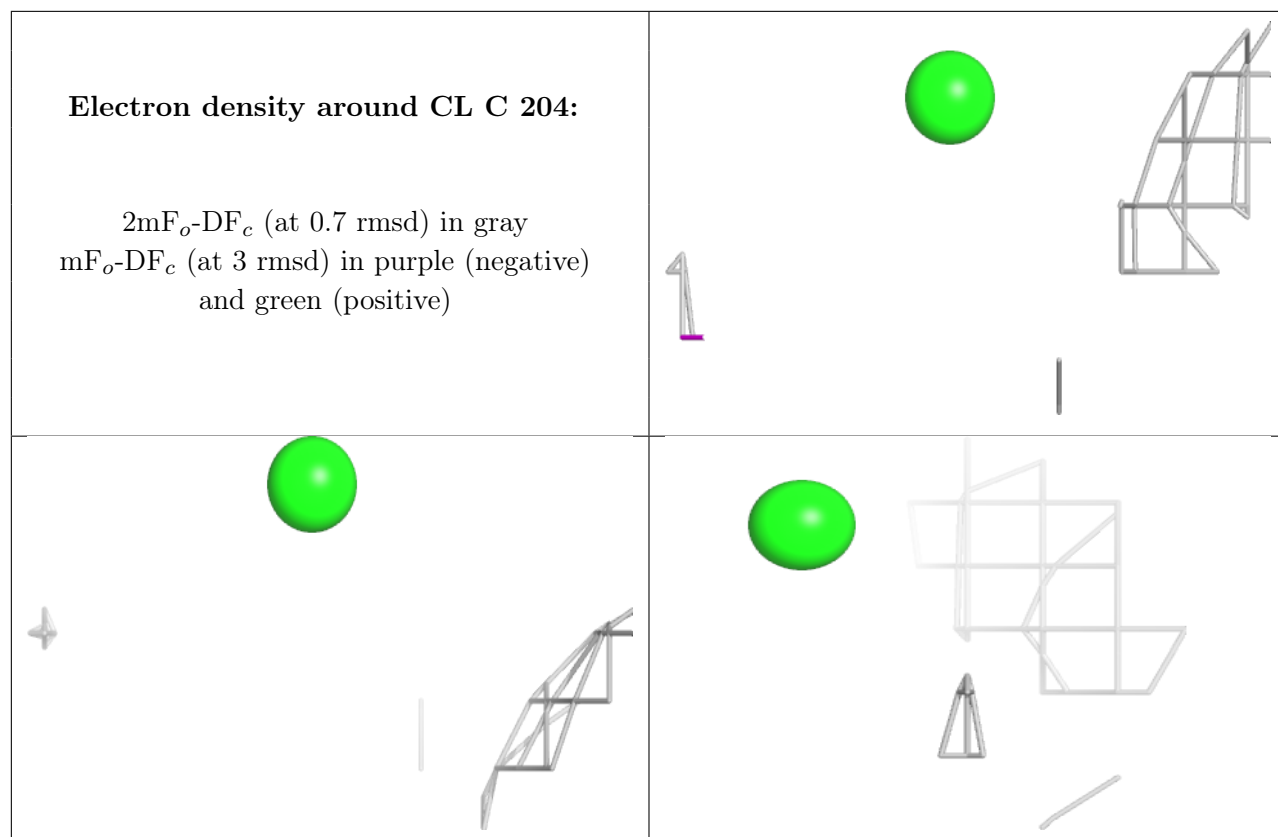
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL H 201:

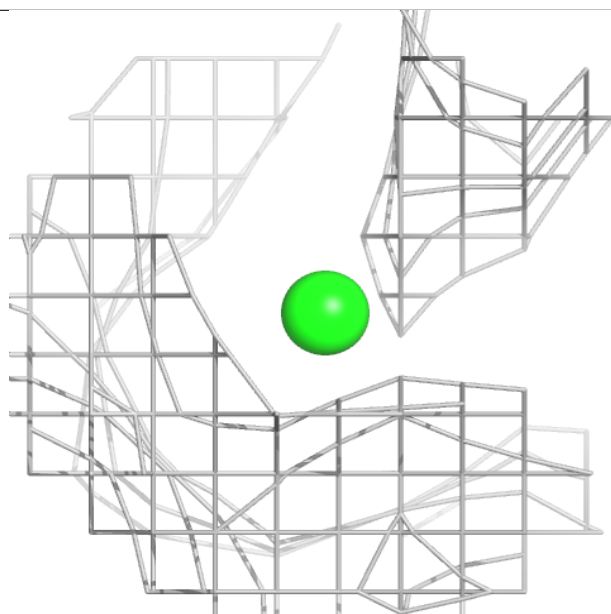
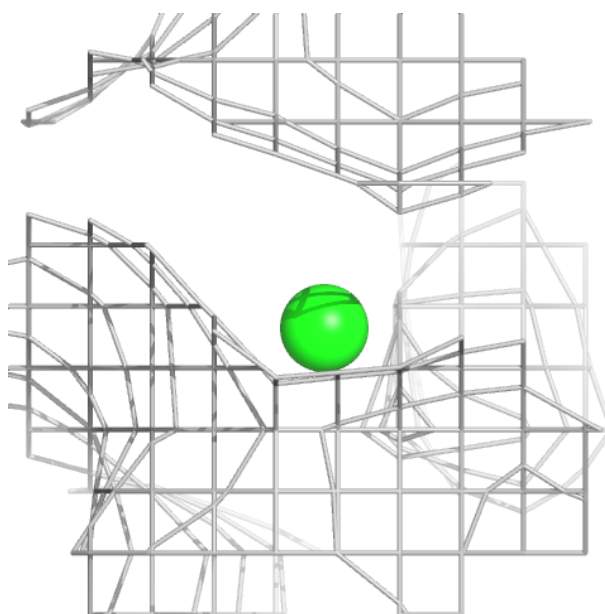
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





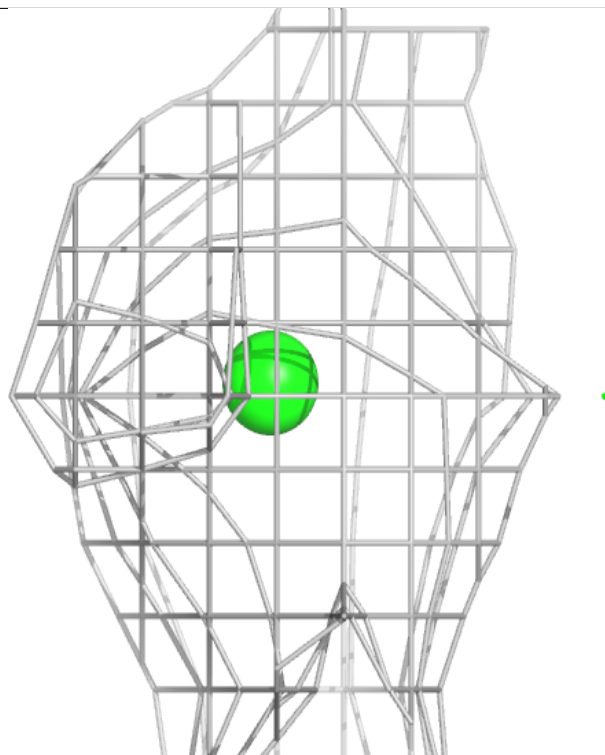
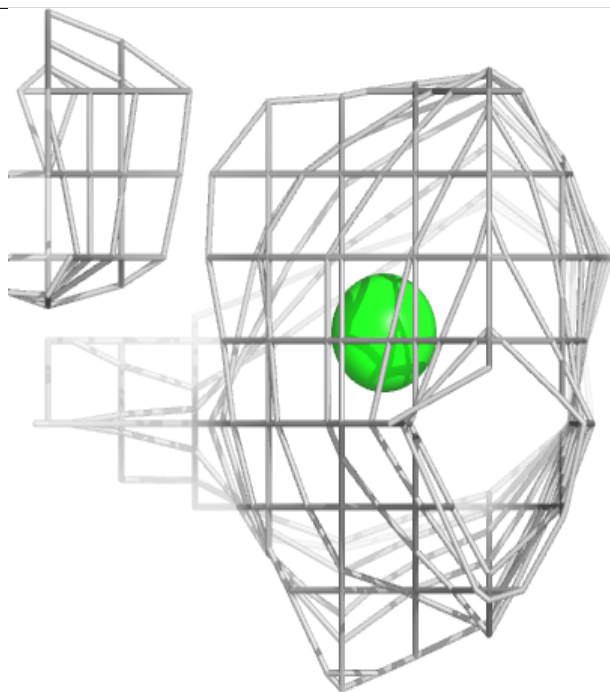
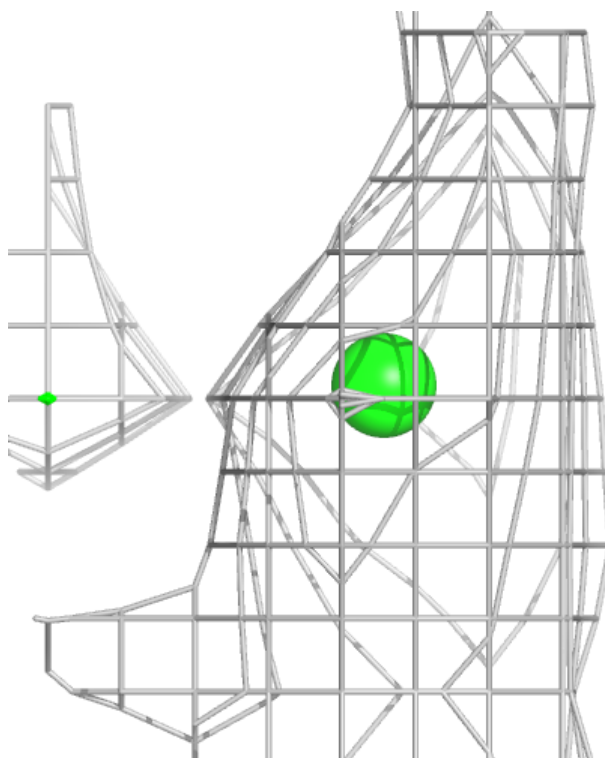
Electron density around CL K 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



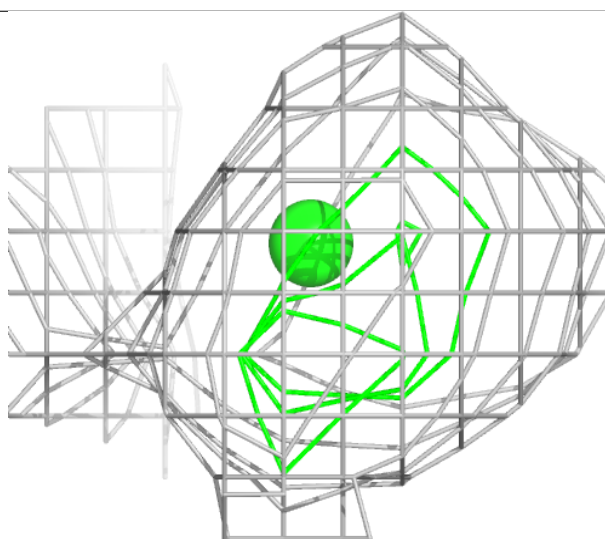
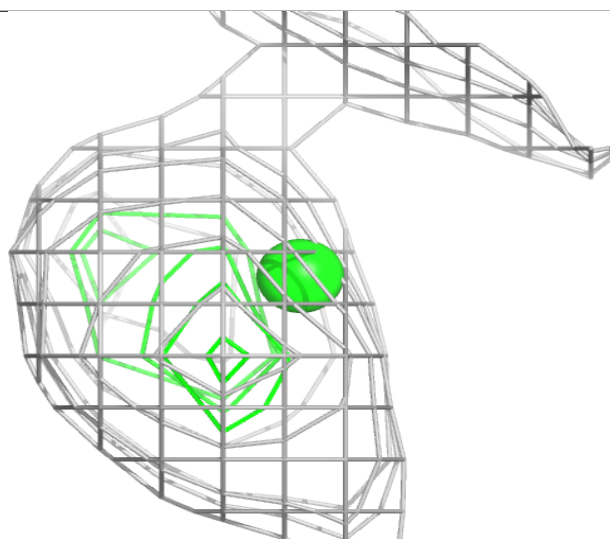
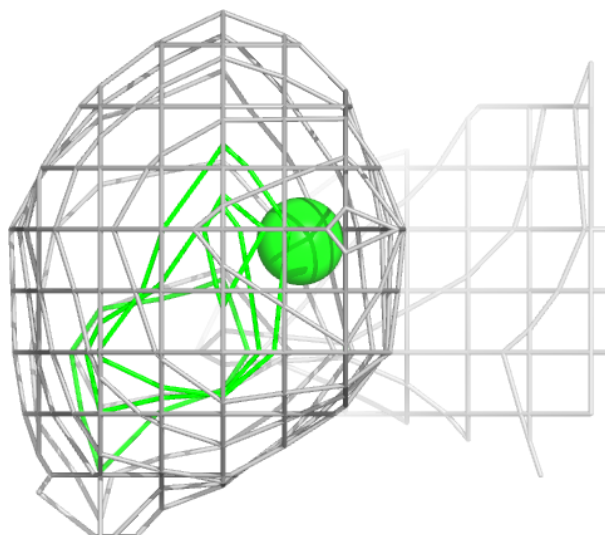
Electron density around CL KK 204:

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and green (positive)



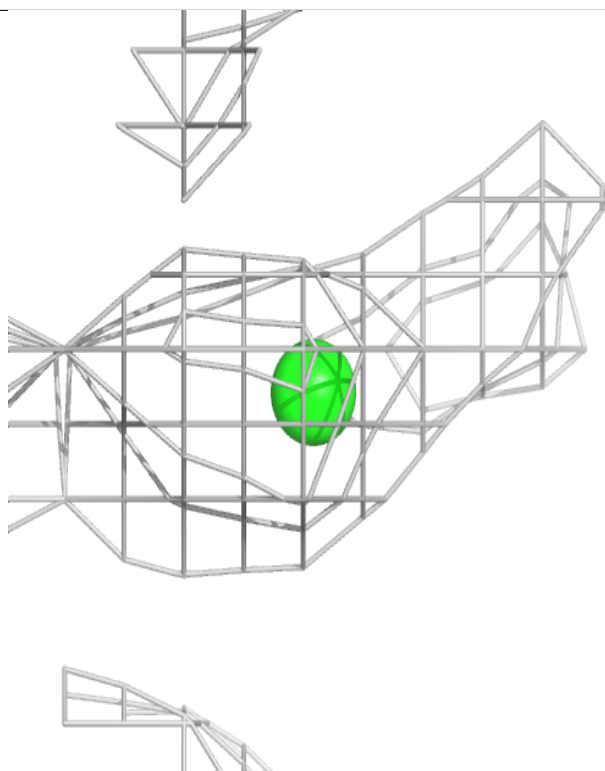
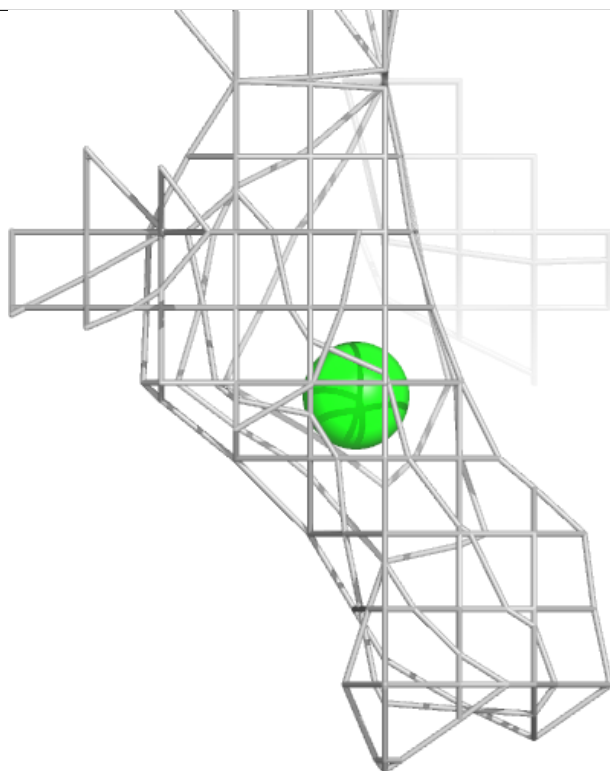
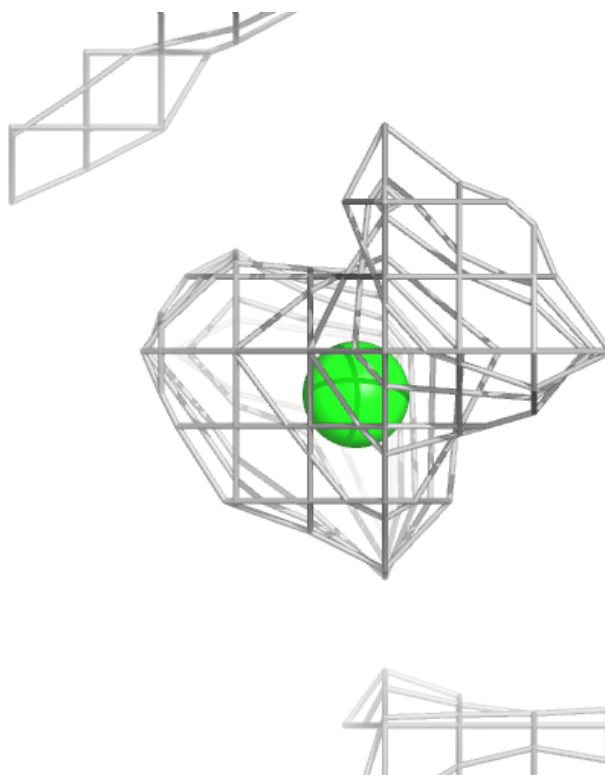
Electron density around CL TT 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



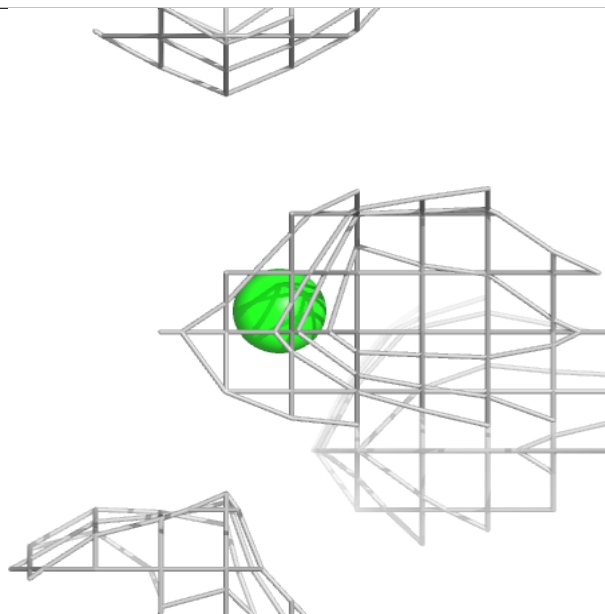
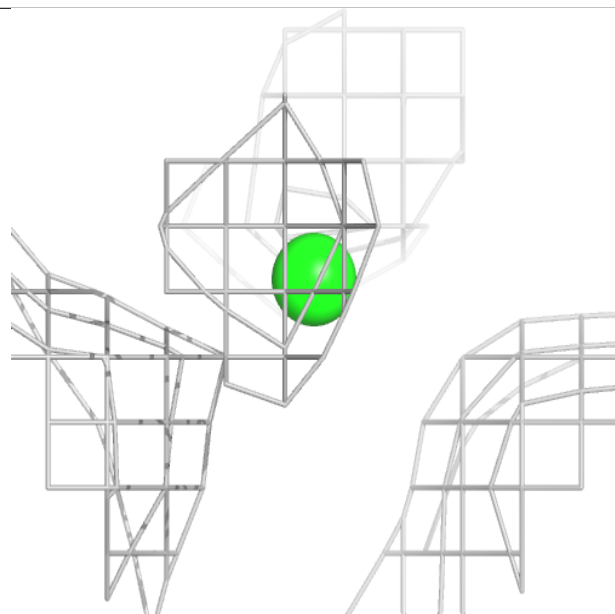
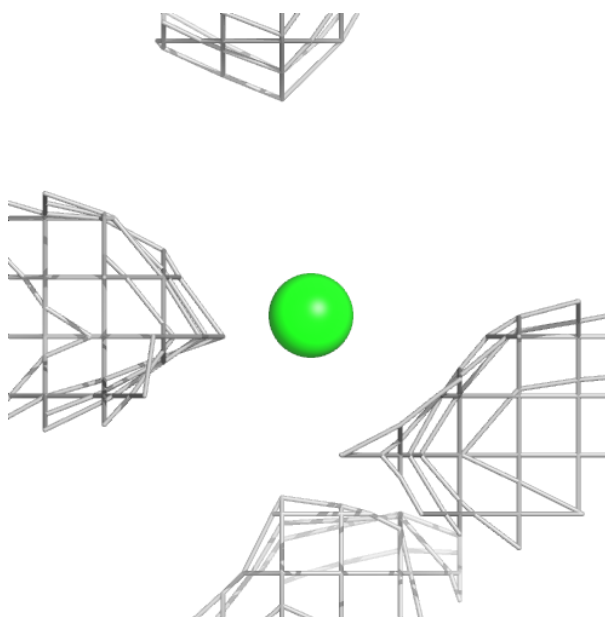
Electron density around CL C 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



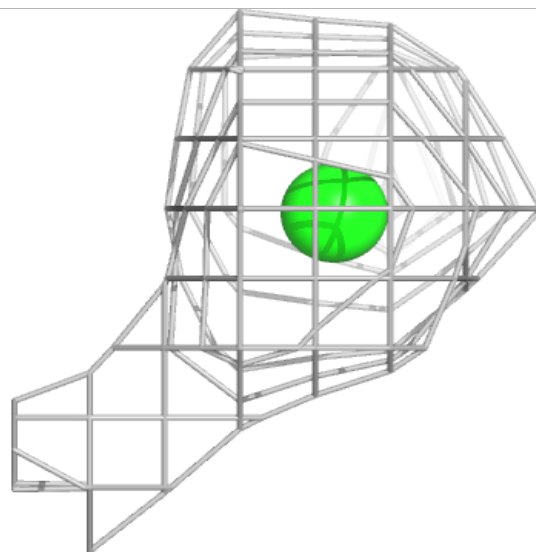
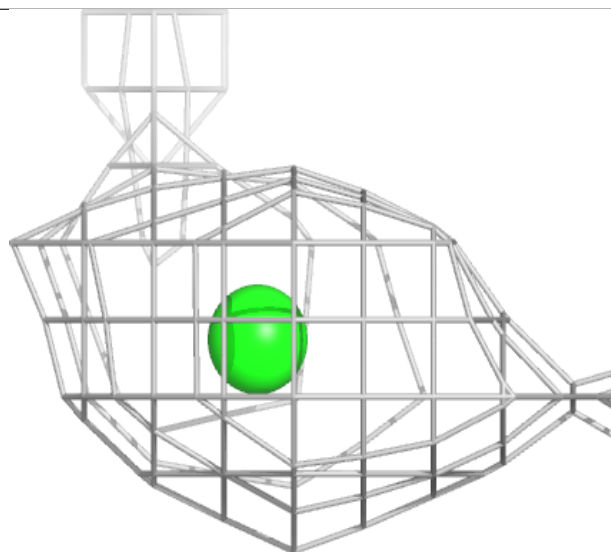
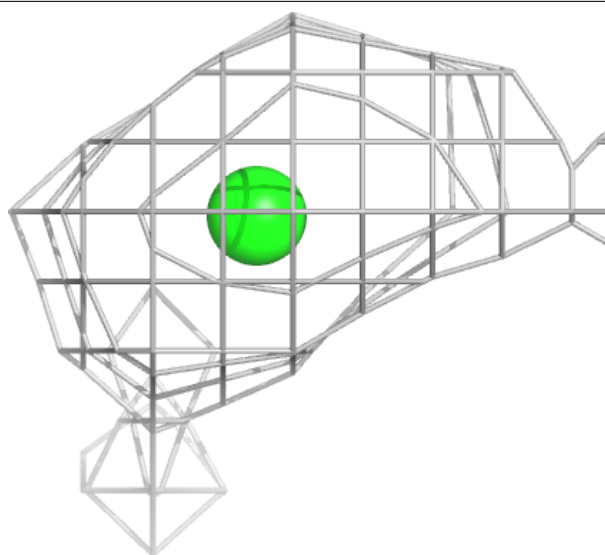
Electron density around CL H 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



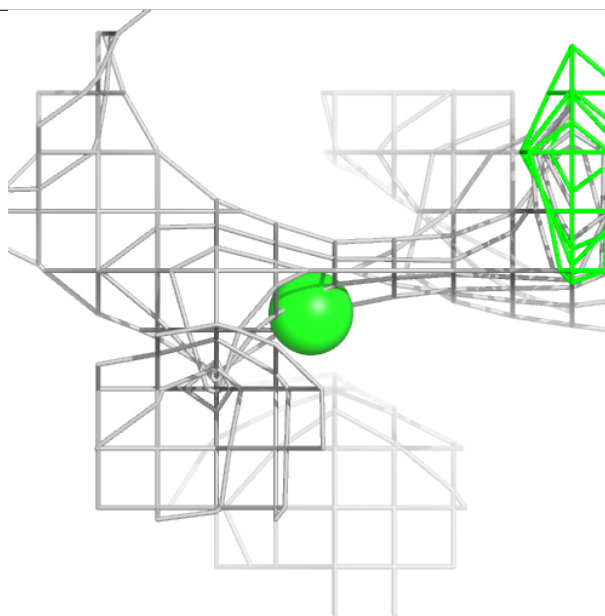
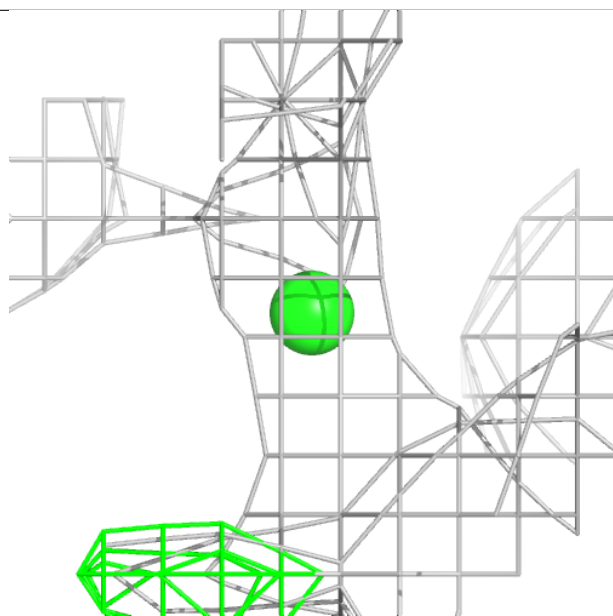
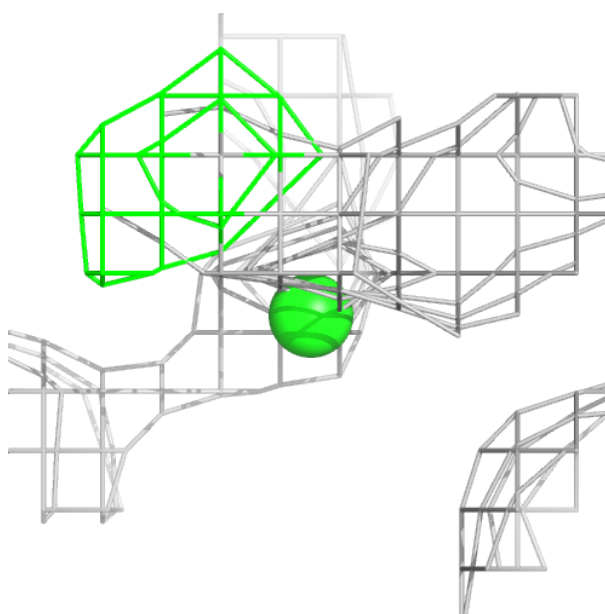
Electron density around CL ll 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



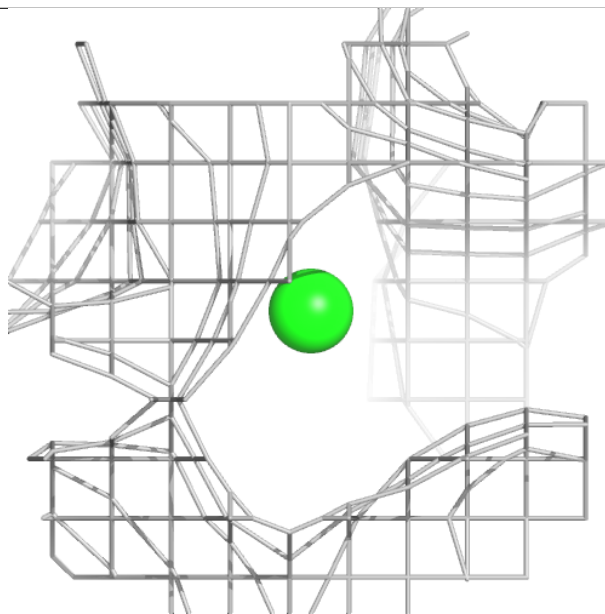
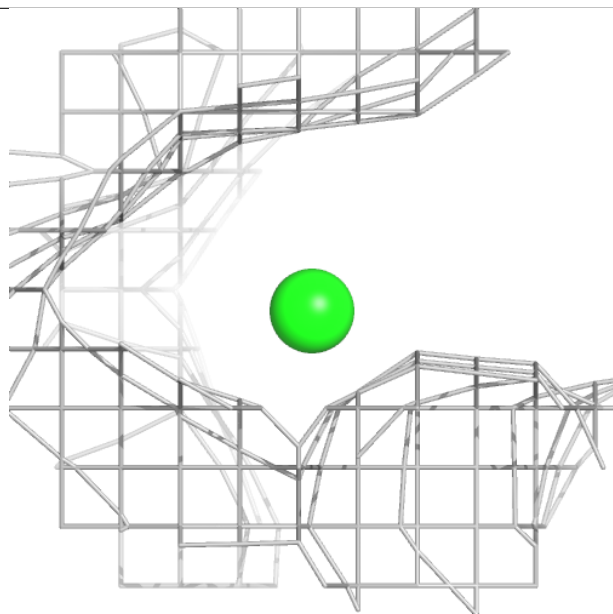
Electron density around CL JJ 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



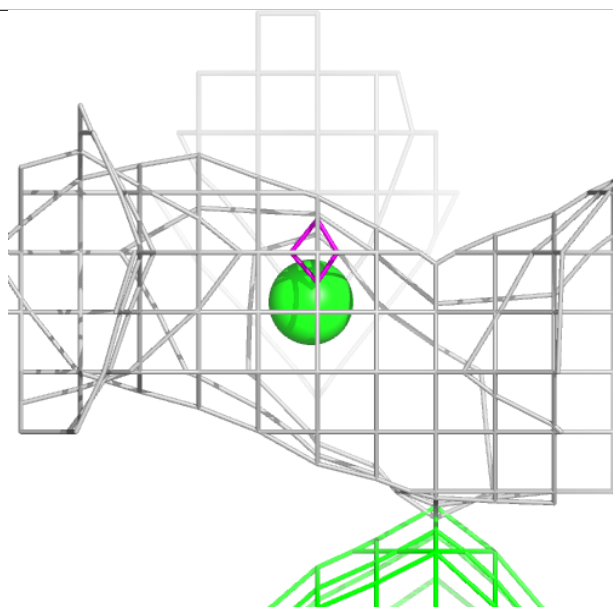
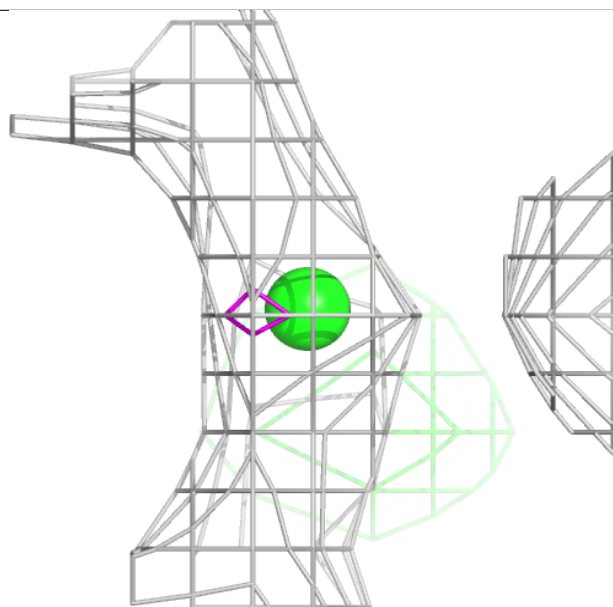
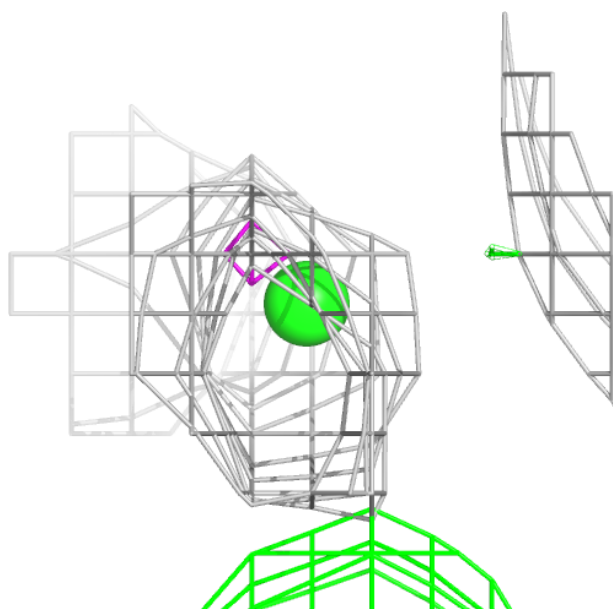
Electron density around CL B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



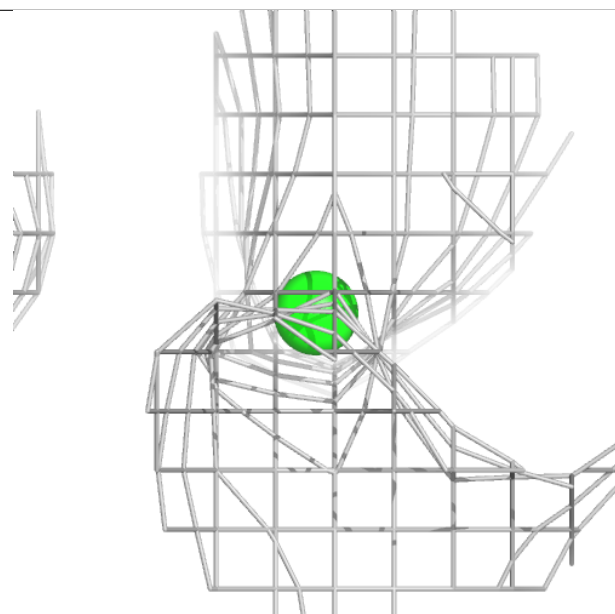
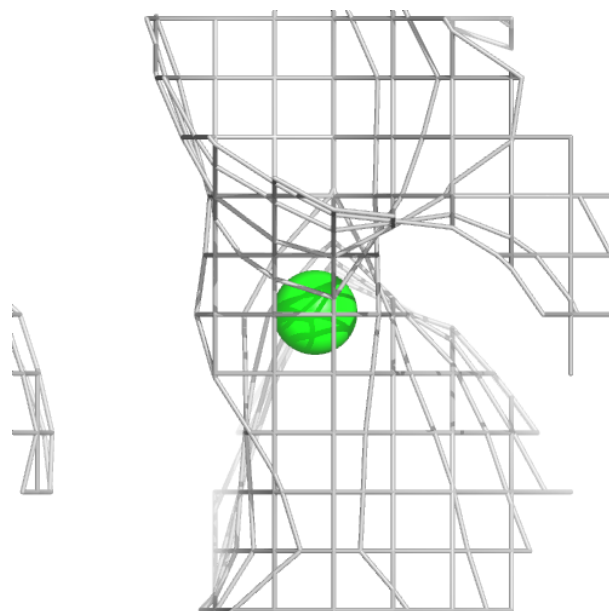
Electron density around CL D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



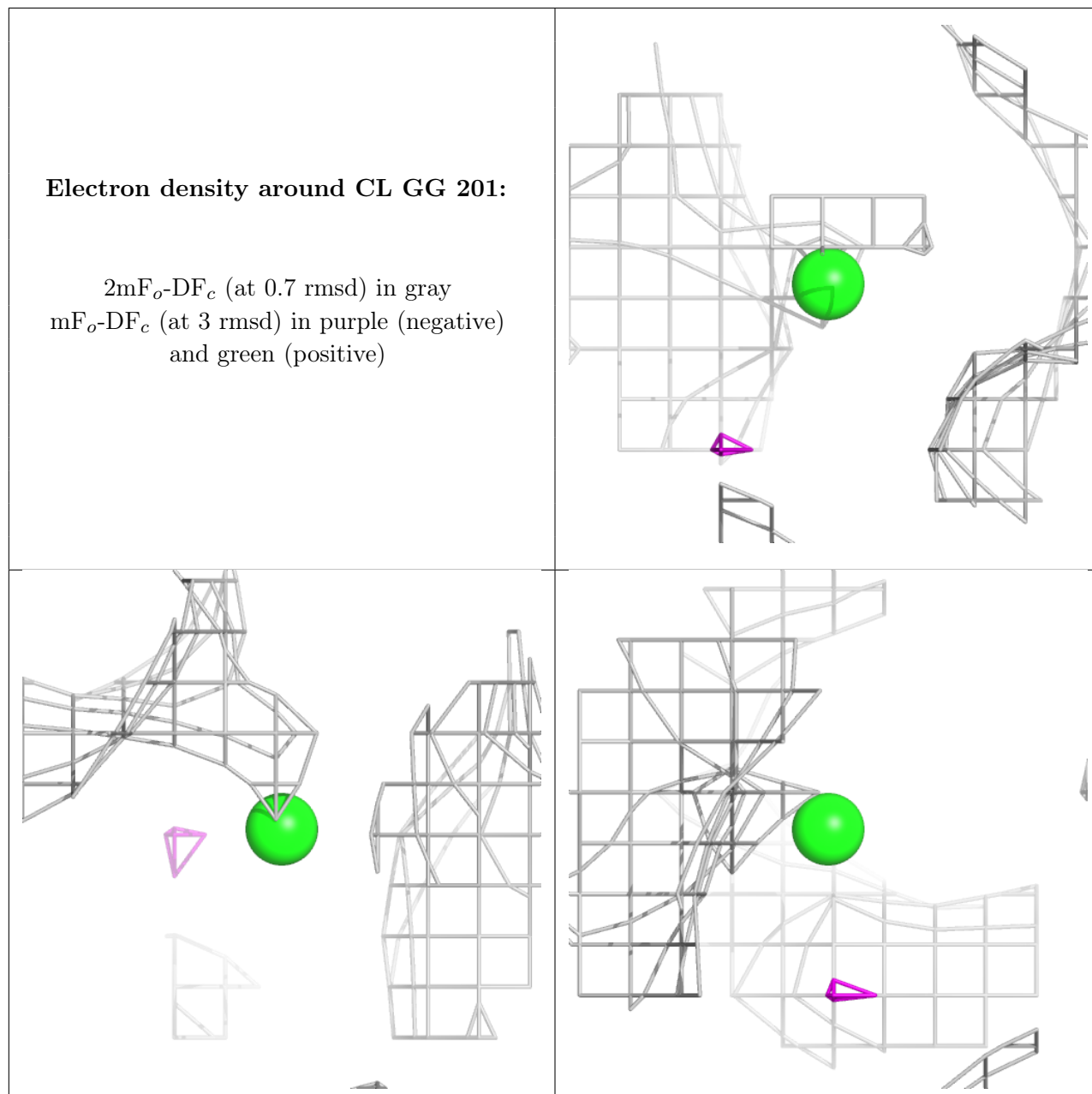
Electron density around CL C 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



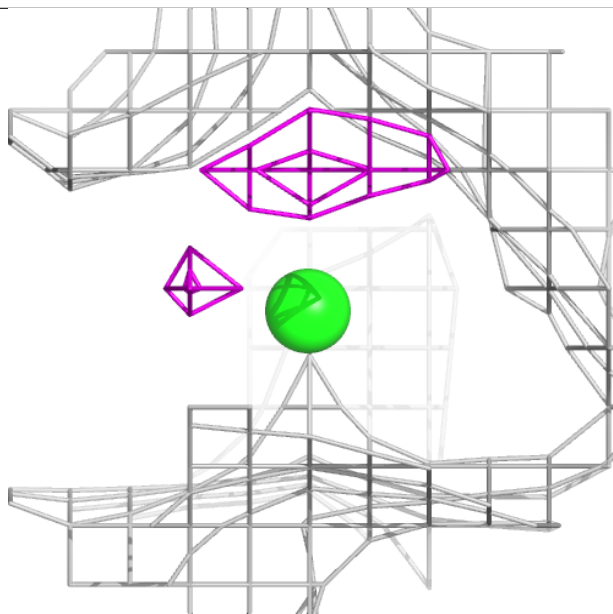
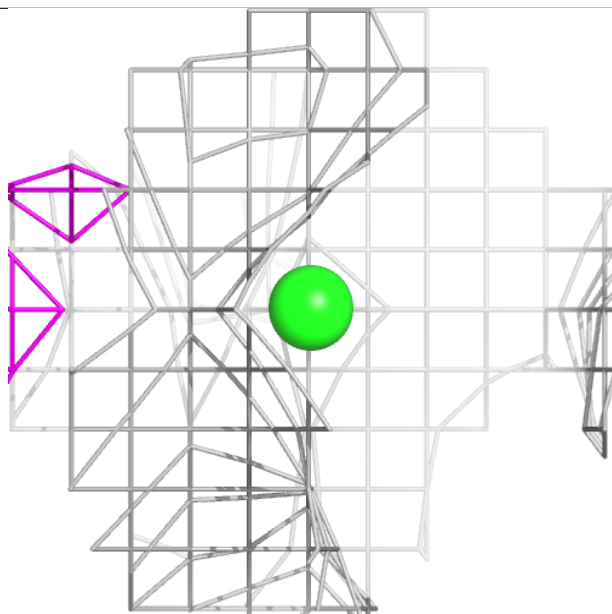
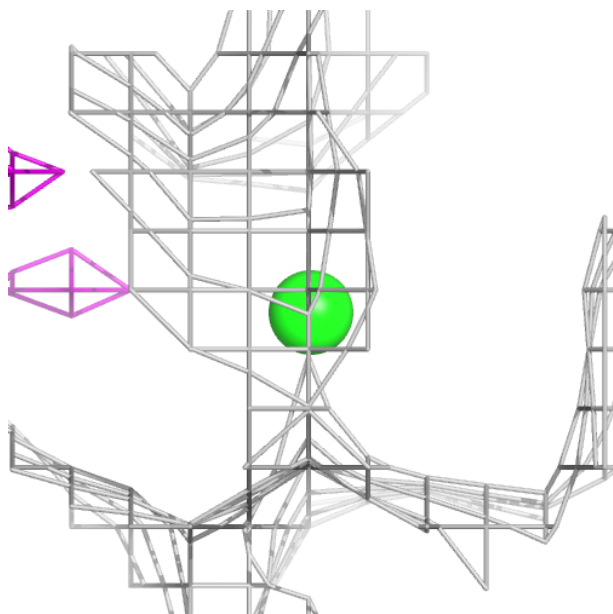
Electron density around CL GG 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



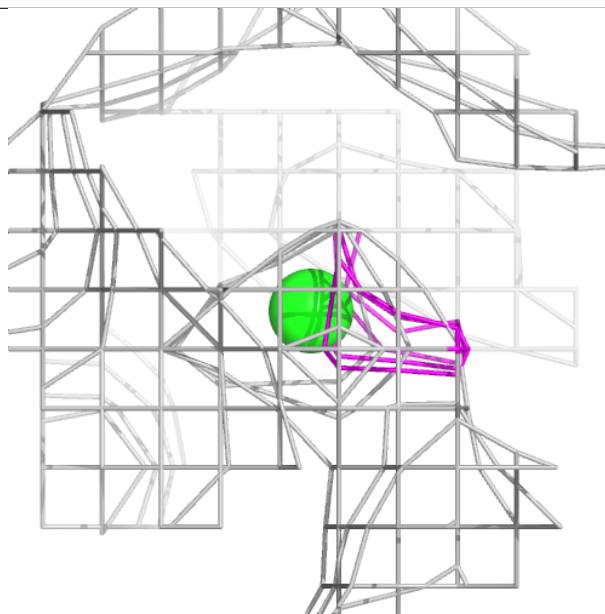
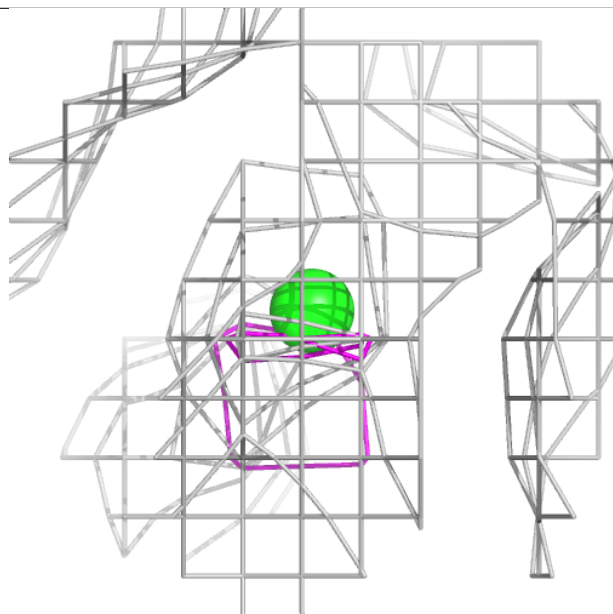
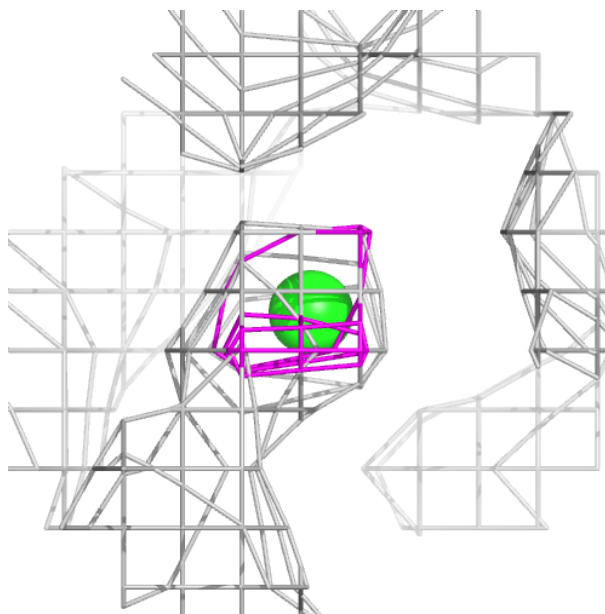
Electron density around CL HH 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



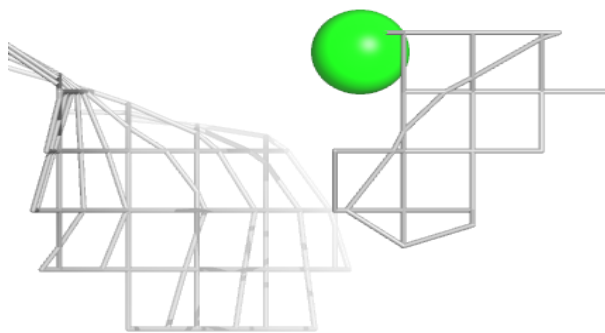
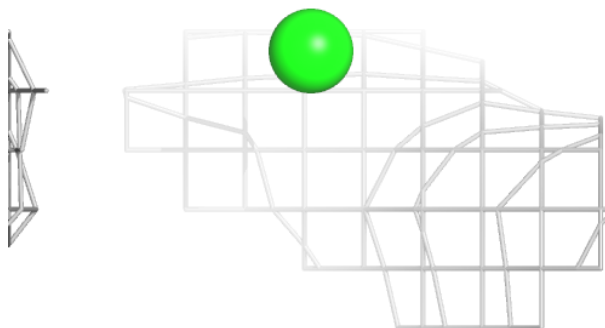
Electron density around CL JJ 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



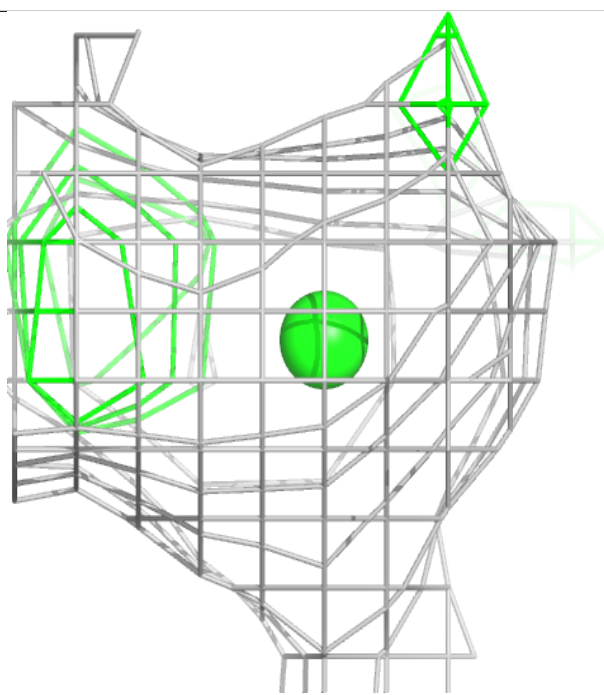
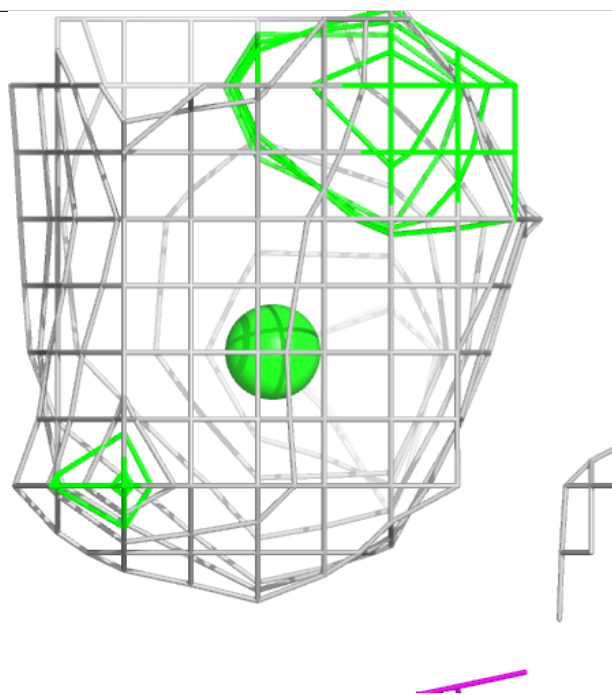
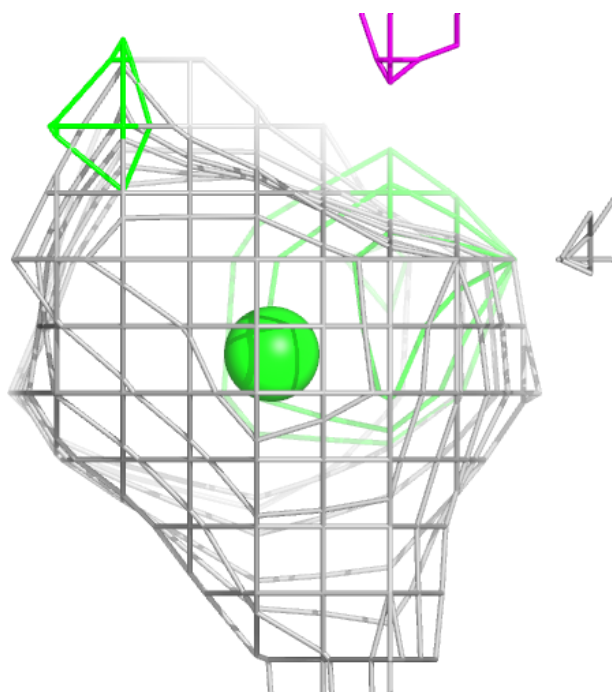
Electron density around CL HH 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



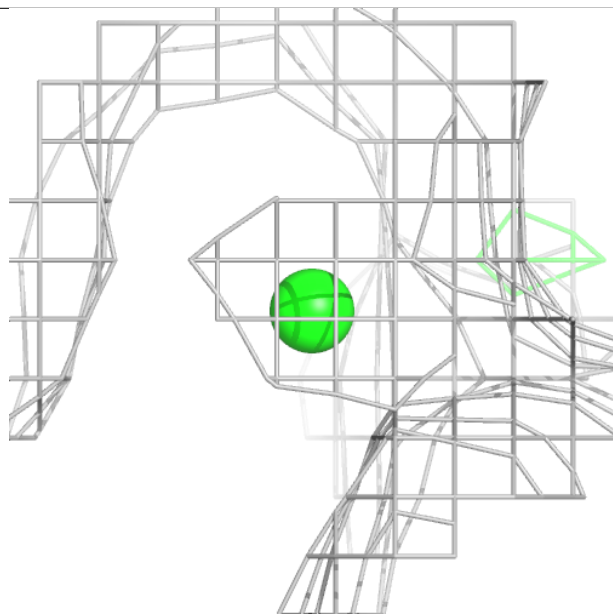
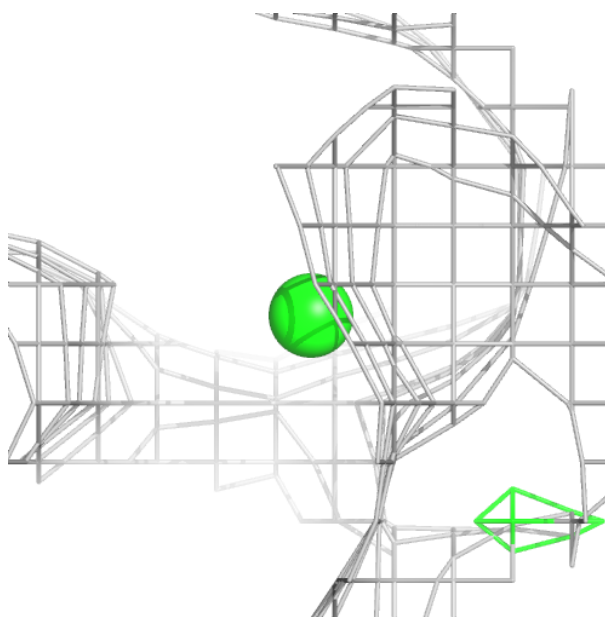
Electron density around CL C 203:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



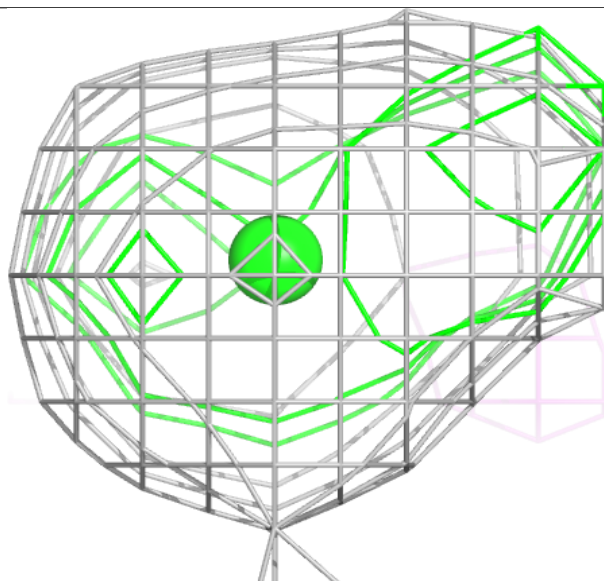
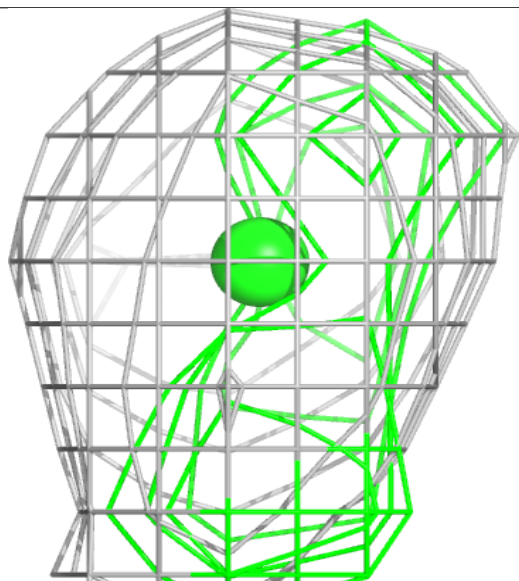
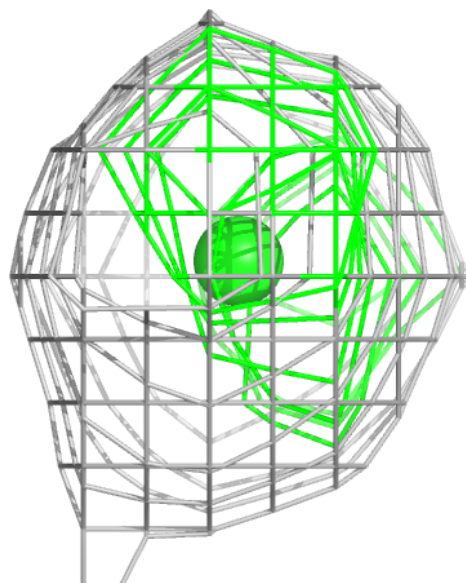
Electron density around CL F 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



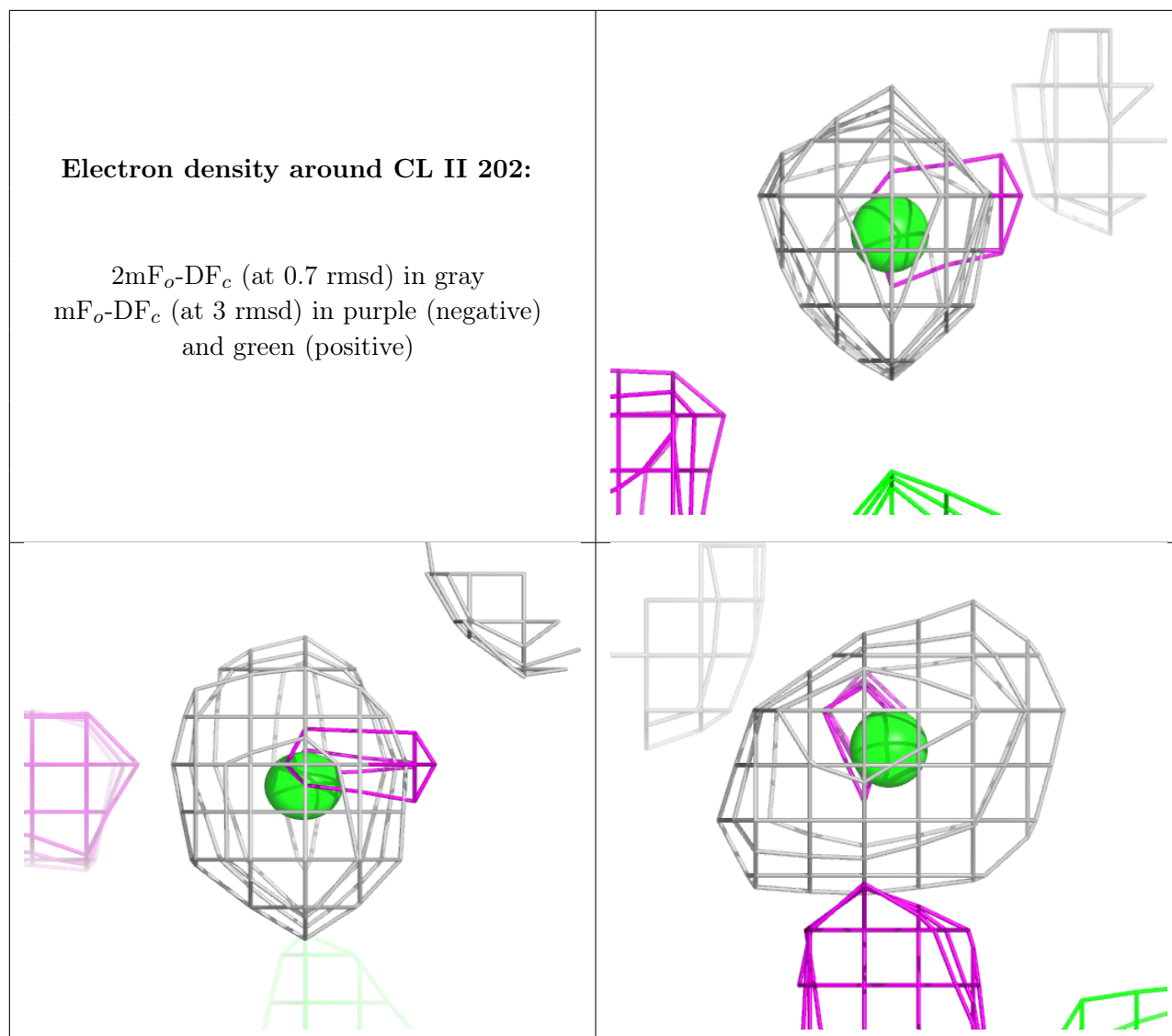
Electron density around CL K 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



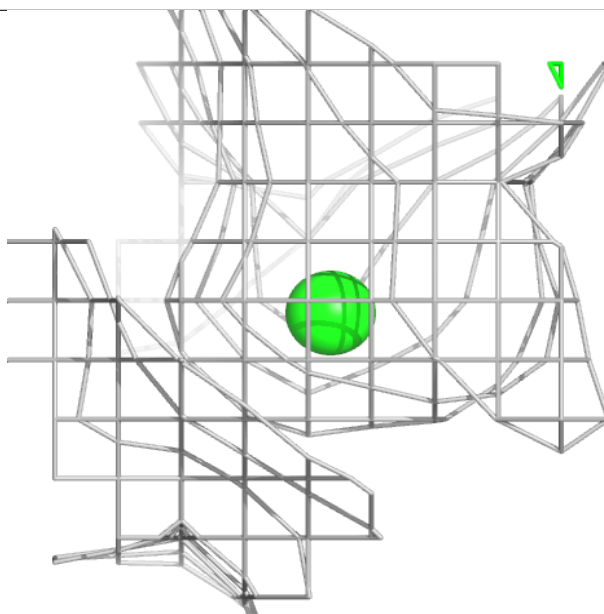
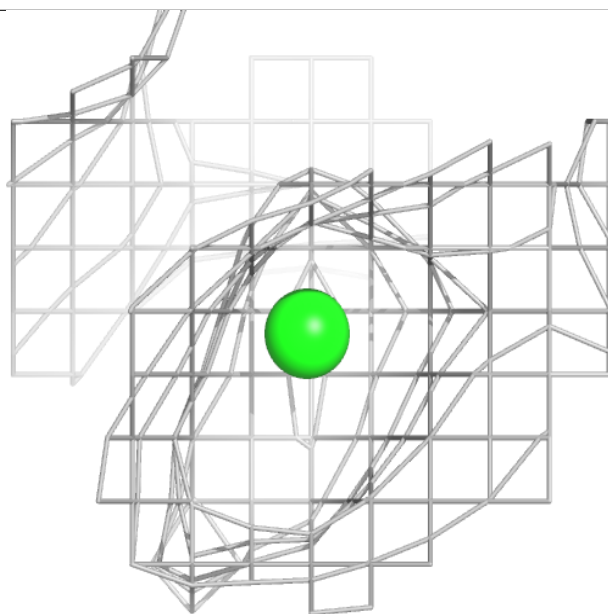
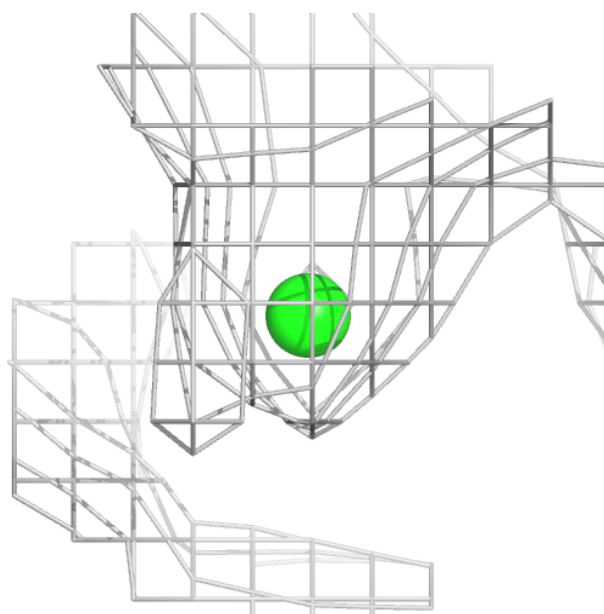
Electron density around CL II 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



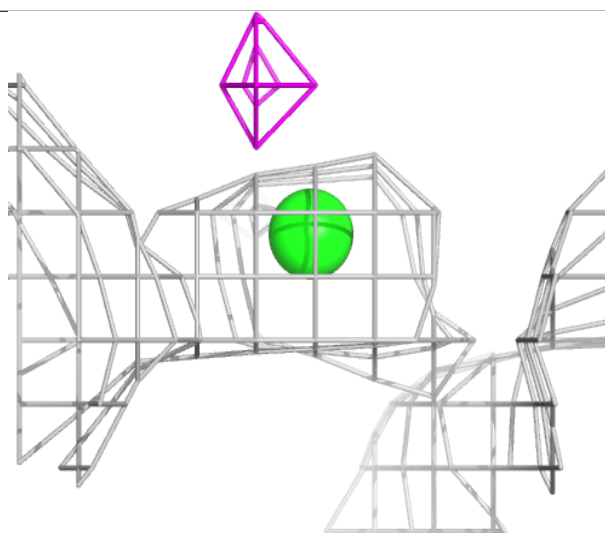
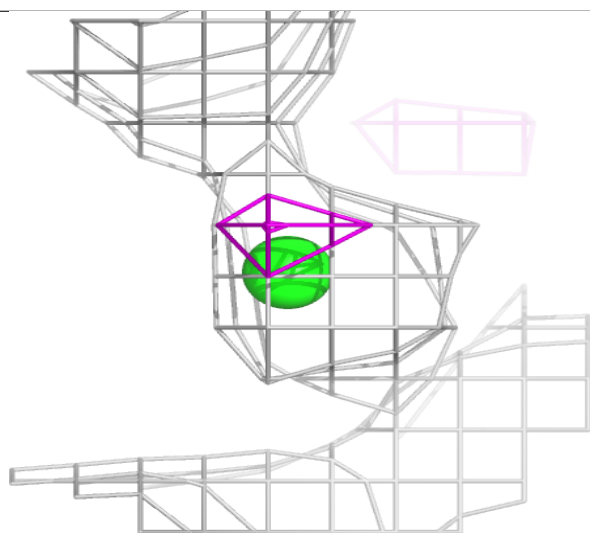
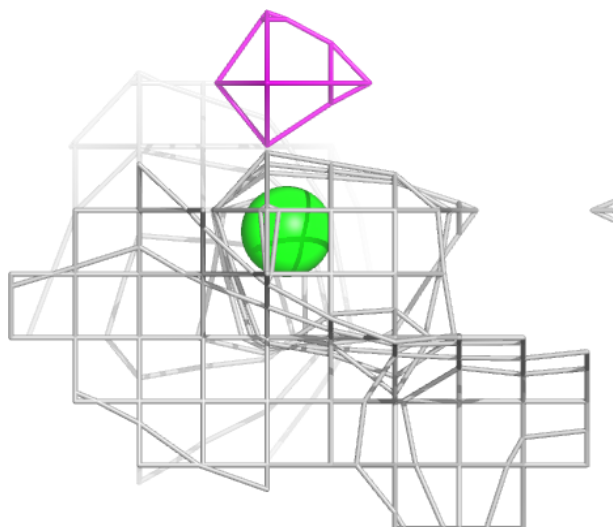
Electron density around CL KK 205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



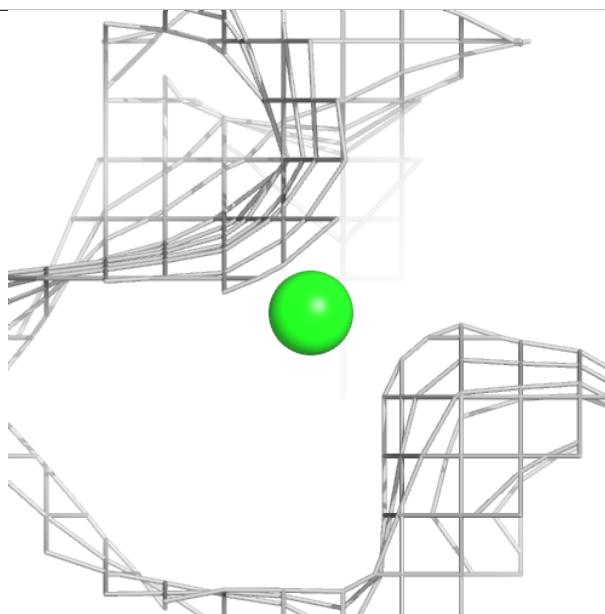
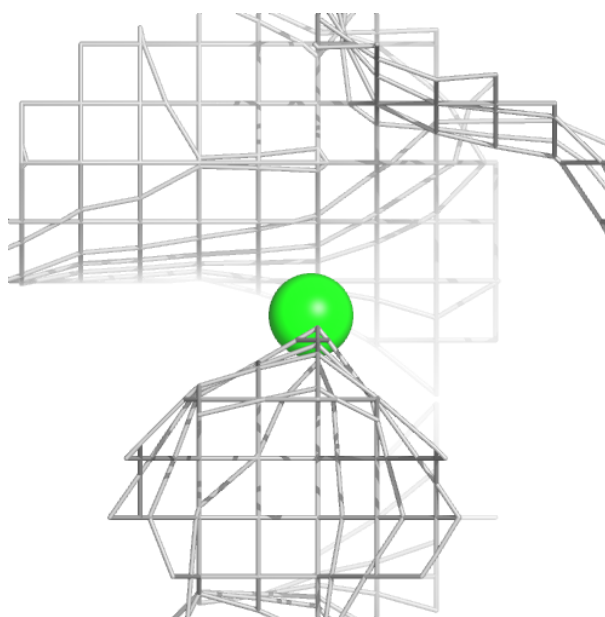
Electron density around CL KK 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



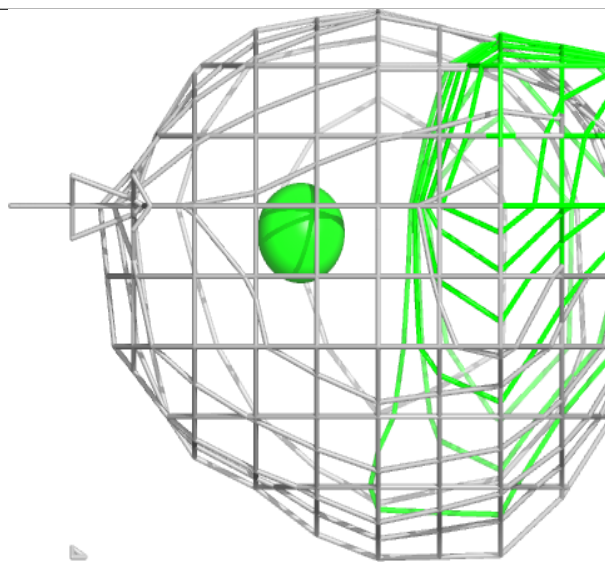
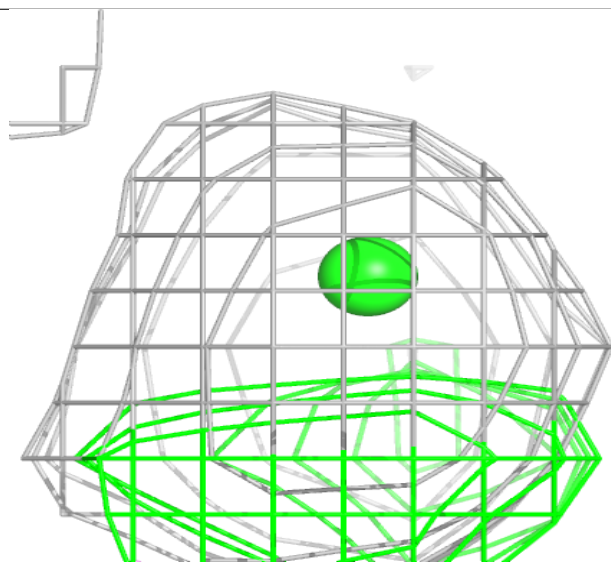
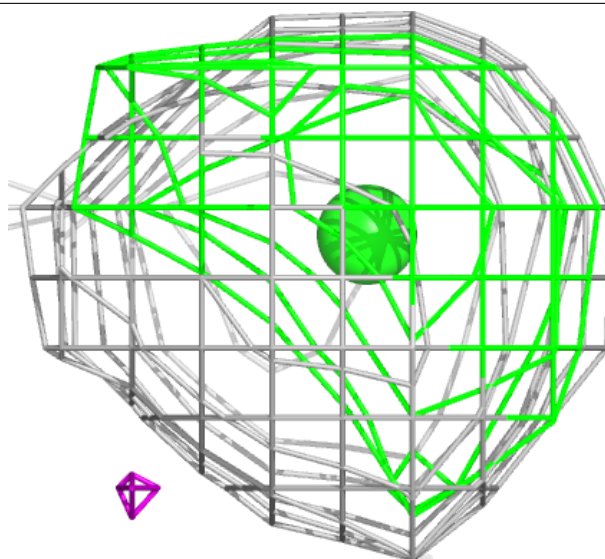
Electron density around CL G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



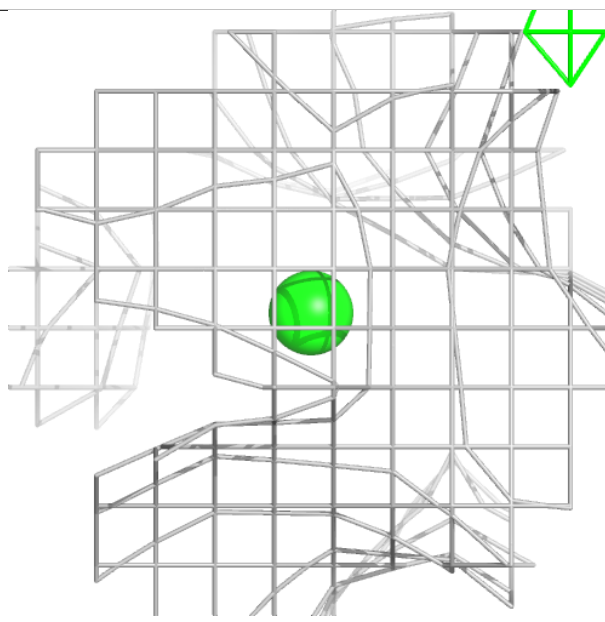
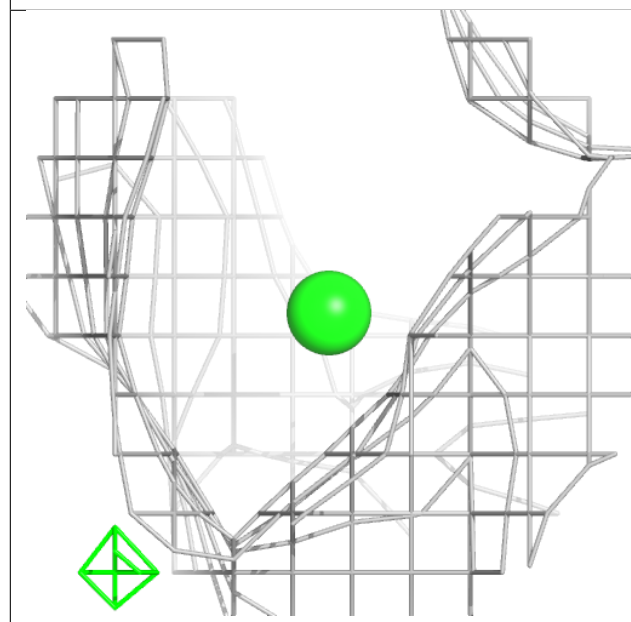
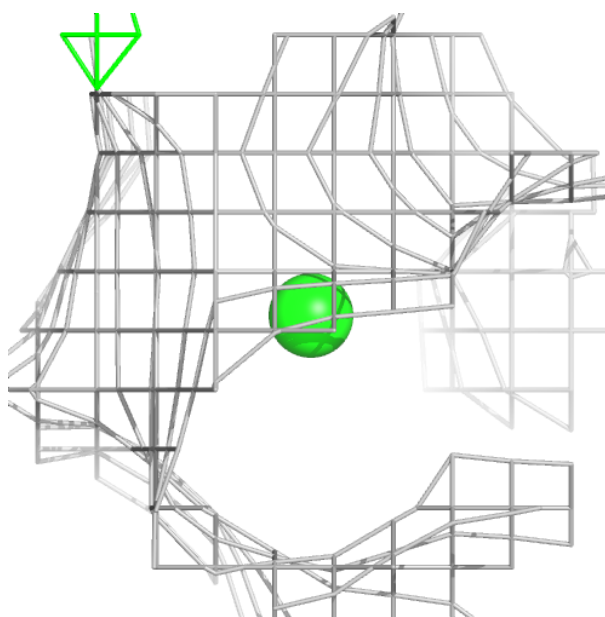
Electron density around CL F 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



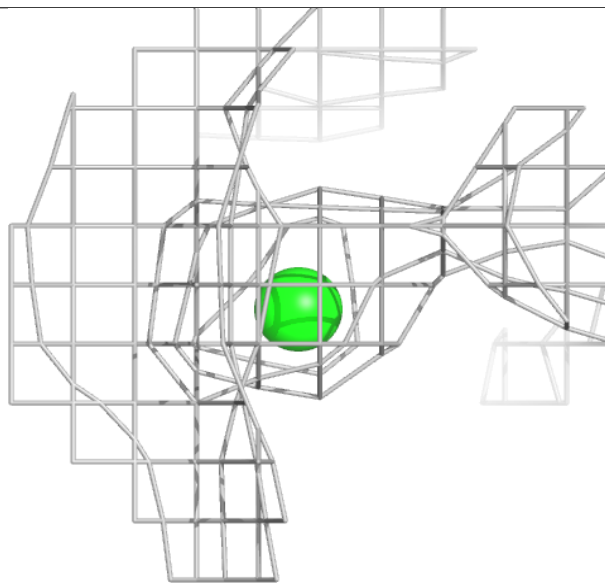
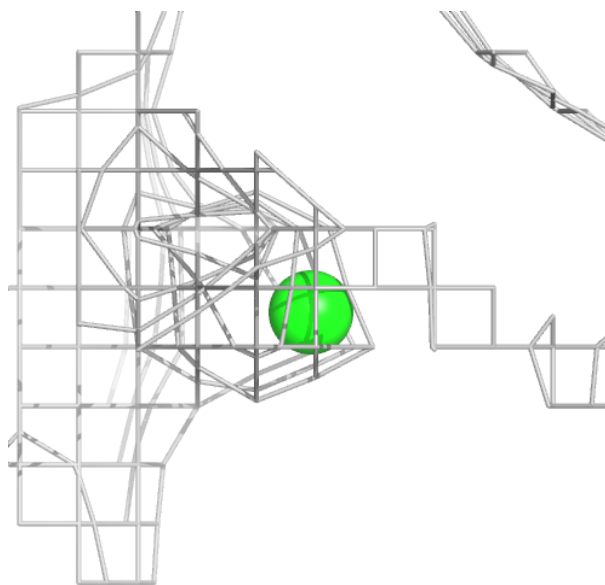
Electron density around CL II 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



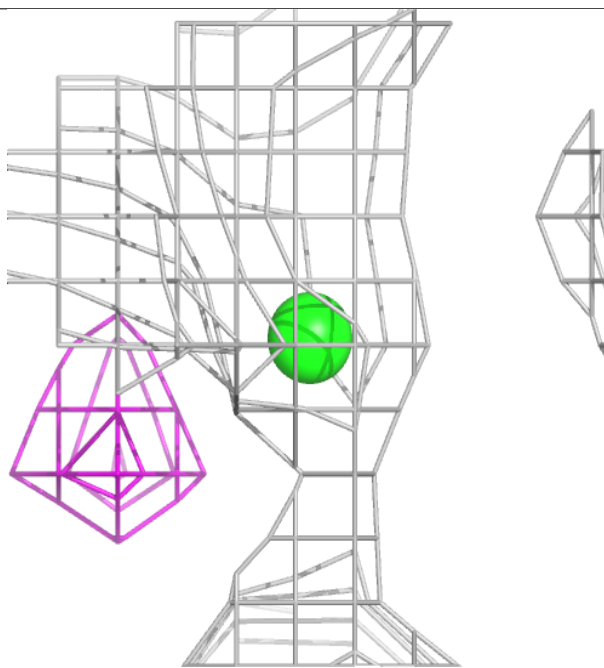
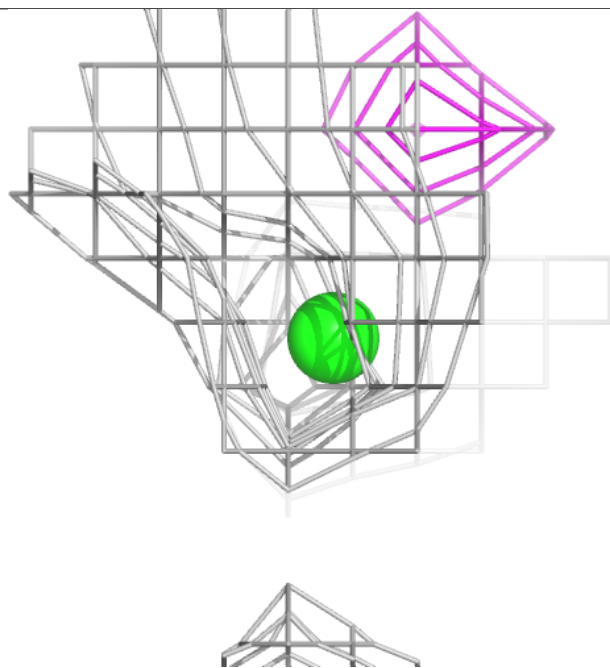
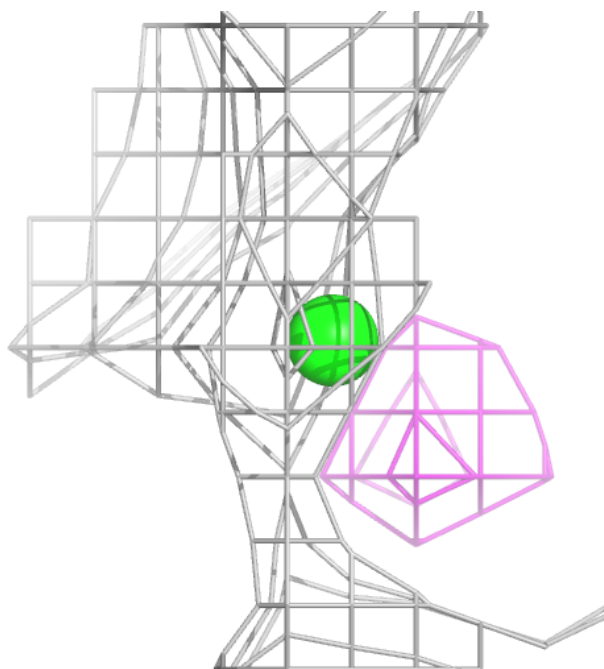
Electron density around CL D 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



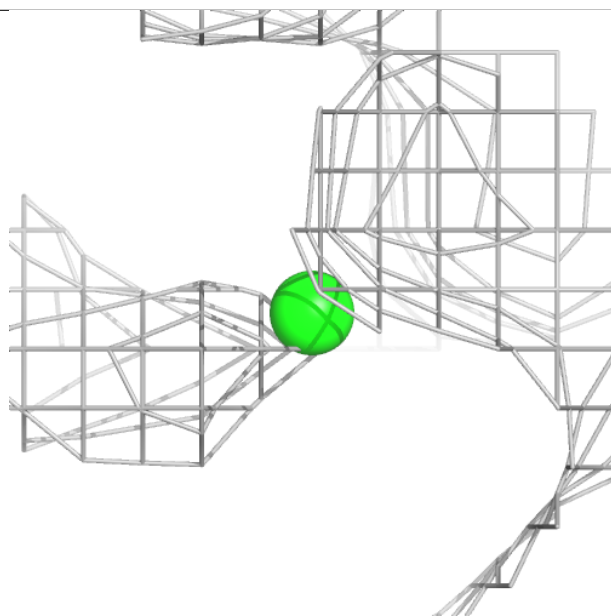
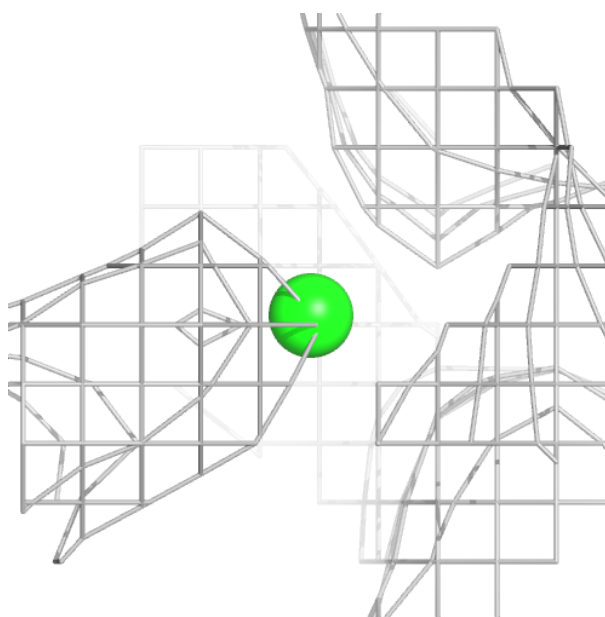
Electron density around CL B 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



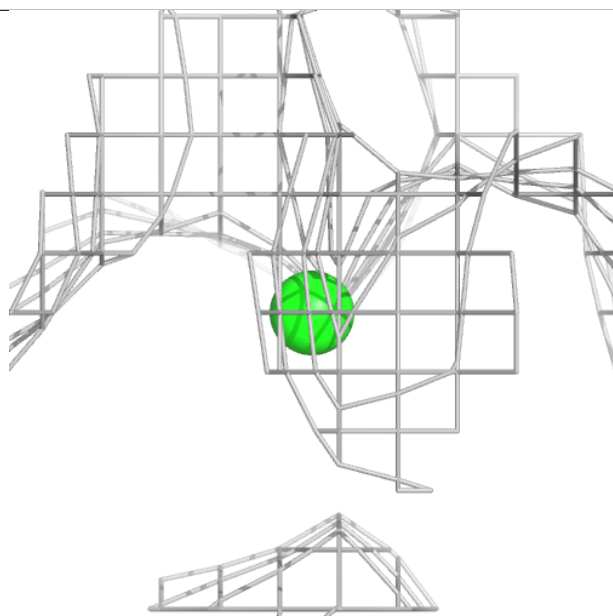
Electron density around CL JJ 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



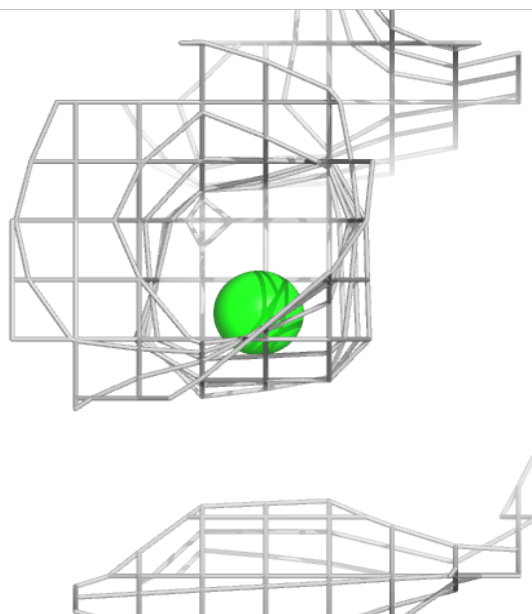
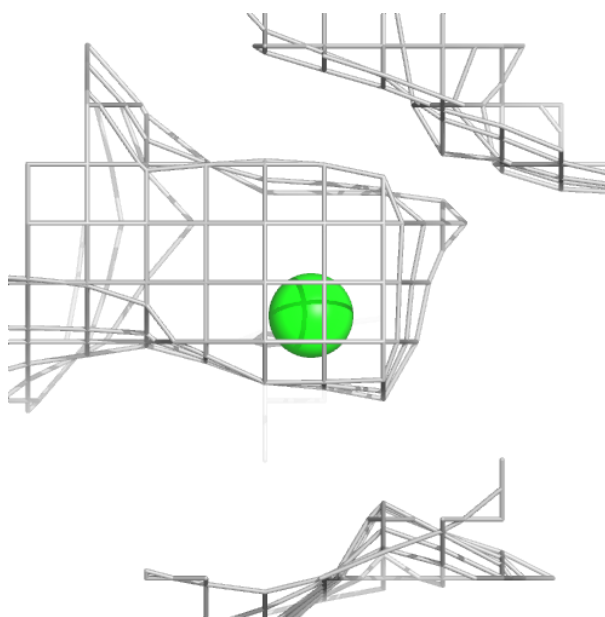
Electron density around CL C 205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



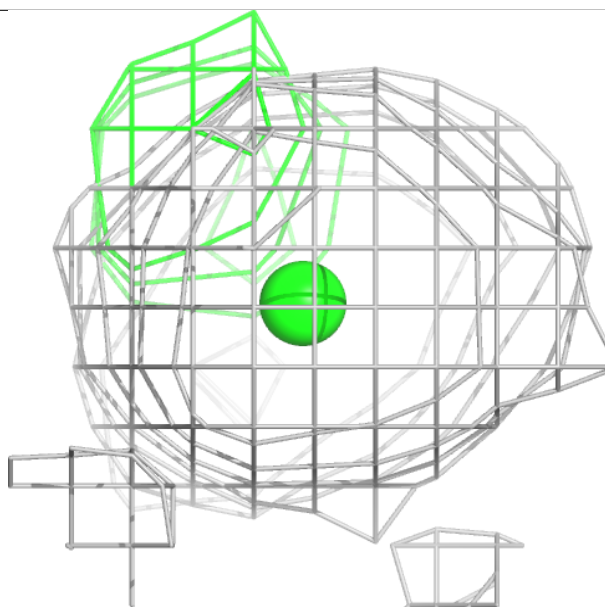
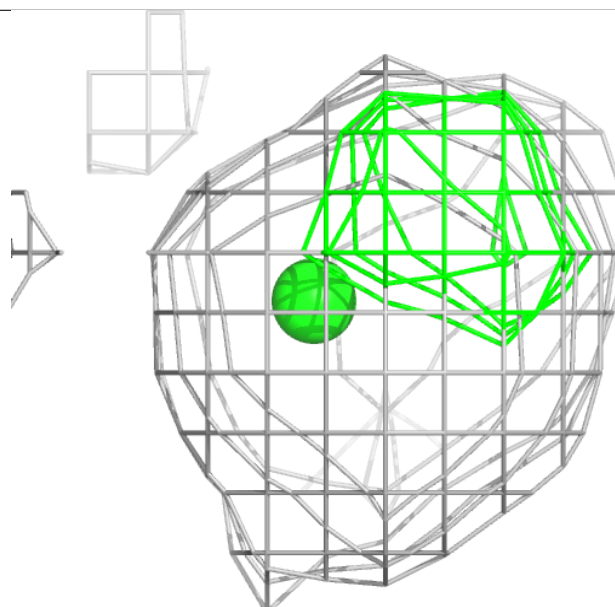
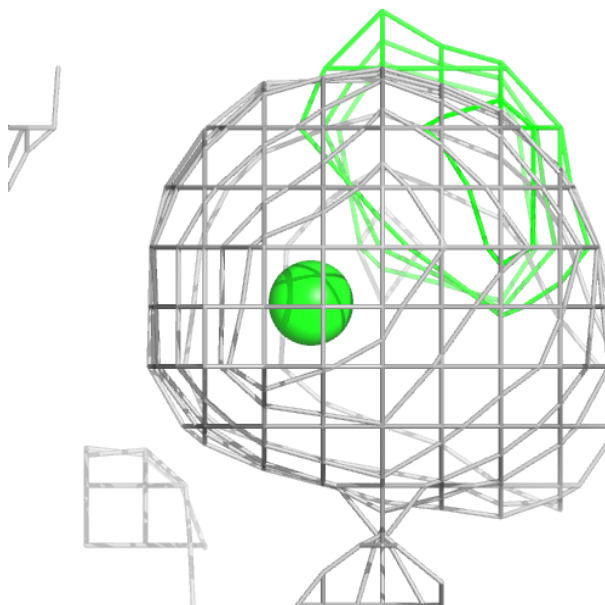
Electron density around CL II 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



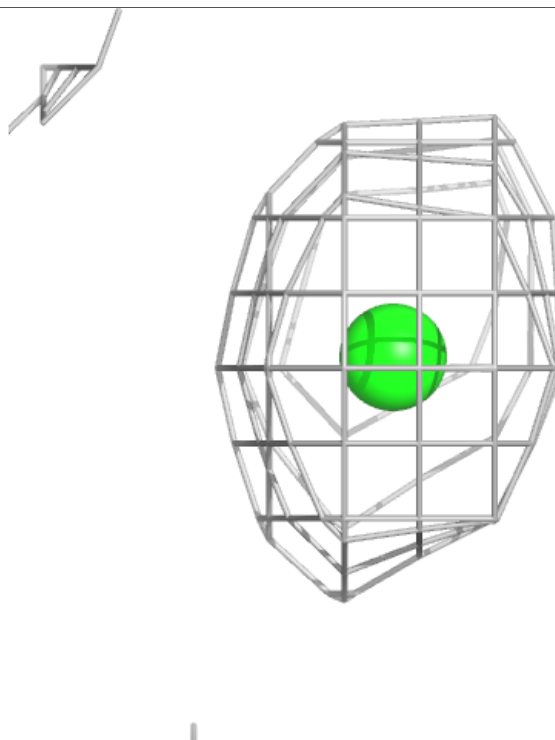
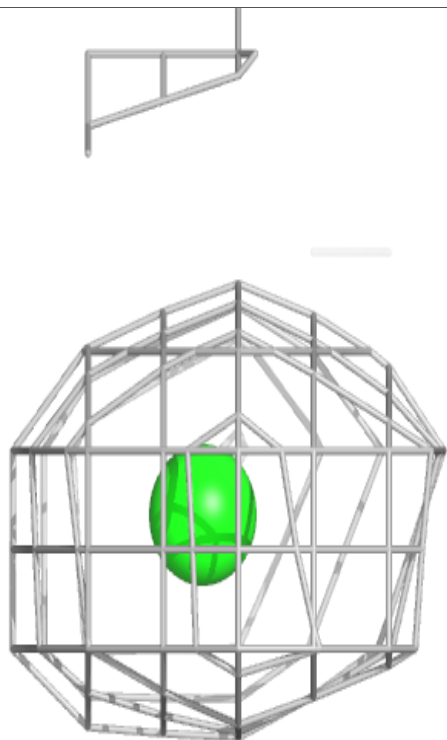
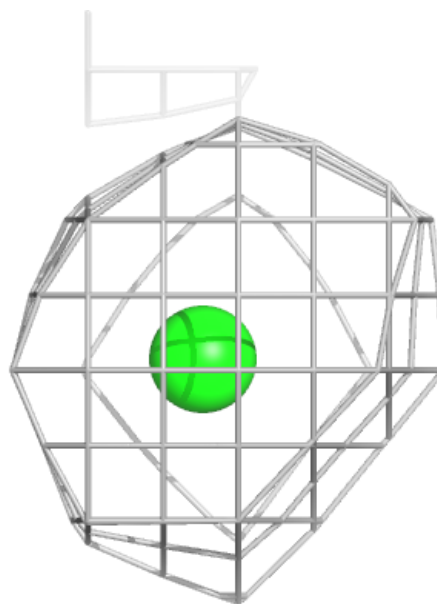
Electron density around CL B 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



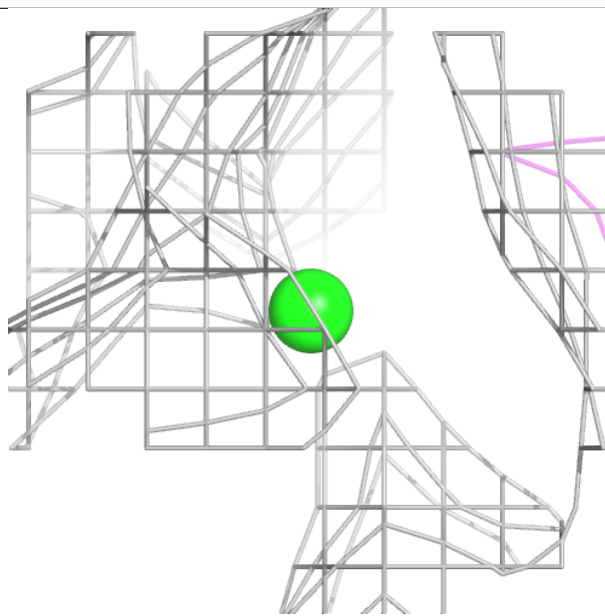
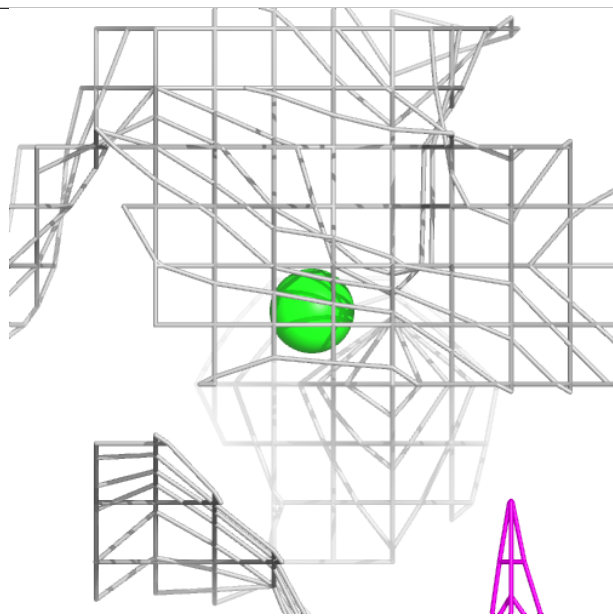
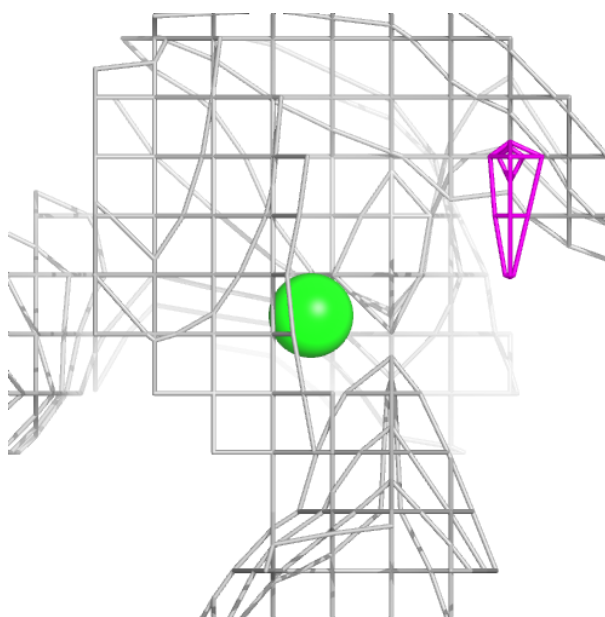
Electron density around CL G 302:

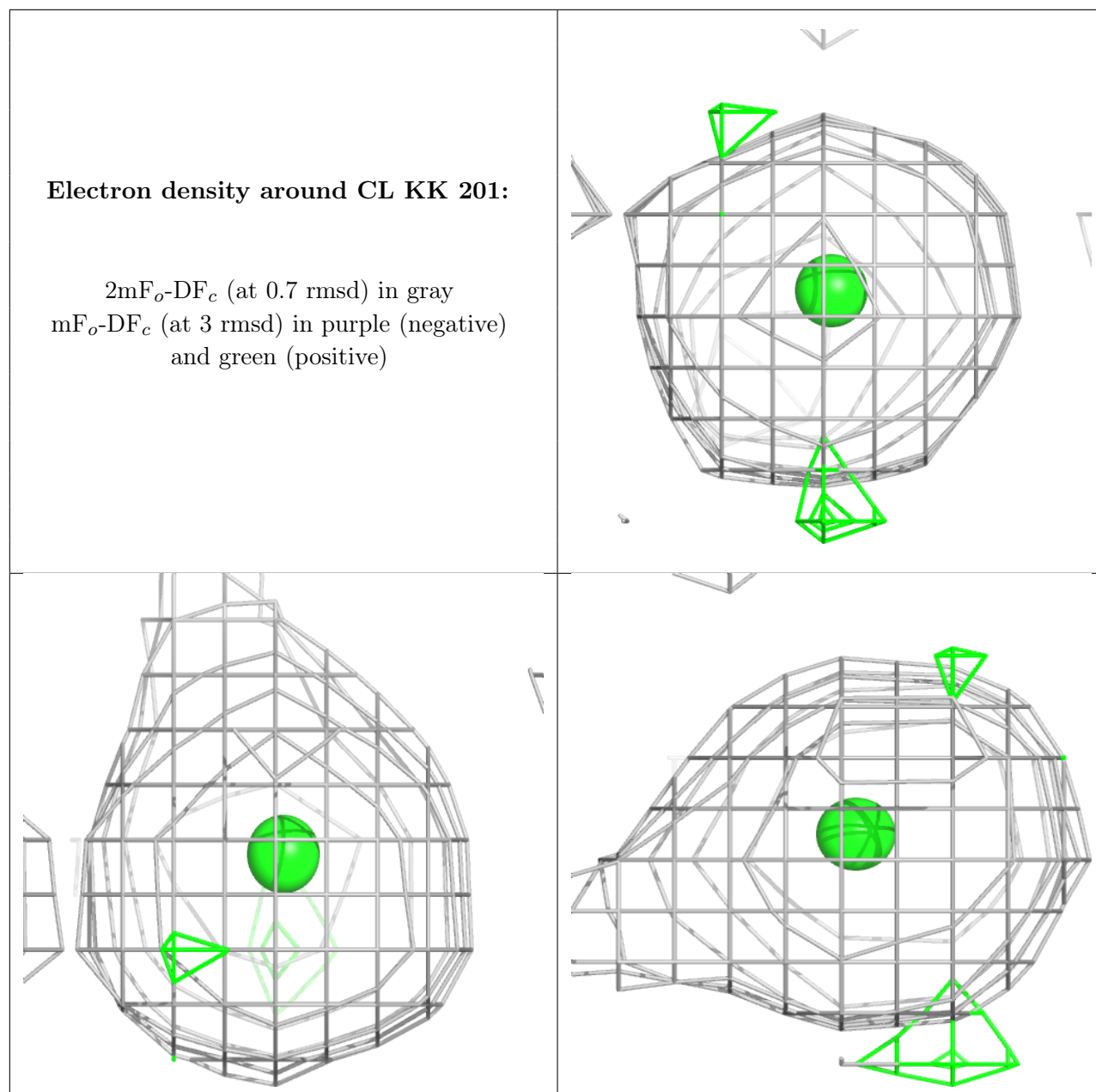
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL C 206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.